Agenzia nazionale per le nuove tecnologie,
l'energia e lo sviluppo economico sostenibile

MINISTERO DELLO SVILUPPO ECONOMICO

Ricerca di Sistema elettrico

RADCAL-III mod. N: calculation of radioactive concentrations in air and at ground level of urban areas located at mesoscale distance (subclass α) from a nuclear plant hit by severe accident - phase 1

Felice De Rosa

Report RdS/PAR2014/135

RADCAL-III MOD. N: CALCULATION OF RADIOACTIVE CONCENTRATIONS IN AIR AND AT GROUND LEVEL OF URBAN AREAS LOCATED AT MESOSCALE DISTANCE (SUBCLASS α) FROM A NUCLEAR PLANT HIT BY SEVERE ACCIDENT - PHASE 1

Felice De Rosa - ENEA

Settembre 2015

Report Ricerca di Sistema Elettrico
Accordo di Programma Ministero dello Sviluppo Economico - ENEA
Piano Annuale di Realizzazione 2014
Area: Produzione di energia elettrica e protezione dell'ambiente
Progetto: Sviluppo competenze scientifiche nel campo della sicurezza nucleare e collaborazione ai programmi internazionali per il nucleare di IV Generazione
Linea: Sviluppo competenze scientifiche nel campo della sicurezza nucleare
Obiettivo: Valutazione degli incidenti e delle loro conseguenze
Responsabile del Progetto: Felice De Rosa, ENEA

Titolo

RADCAL-III mod.N: Calculation of radioactive concentrations in air and at ground level of urban areas located at mesoscale distance (subclass α) from a nuclear plant hit by severe accident - phase 1

Descrittori

Tipologia del documento:

Collocazione contrattuale: Accordo di programma ENEA-MSE: Piano Annuale di Realizzazione 2014, Linea Progettuale 1, Obiettivo B: Valutazione degli incidenti e delle loro conseguenze, Task B2, Tema 2.

Argomenti trattati: Analisi incidentale, Codici e modelli avanzati per il calcolo delle concentrazioni in aria e al suolo a seguito di rilasci radioattivi da centrali nucleari causati da incidente grave.

Sommario

This report describes the activities performed in the frame of LP1, Objective B, task B2, theme 2 of PAR-2014. The Ministry of Economic Development (MiSE), through the B.3.1. Program agreement with ENEA, have funded two project lines in the field of nuclear energy. The first one is aimed at maintaining and, where applicable, to increase the growth of a system of scientific expertise dedicated to safety, security and sustainability of nuclear power, in order to be ready for independent safety assessments in the case of emergencies caused by severe accidents in NPPs located near the Italian border. RADCAL-III mod. N is a code under development and validation, characterized by innovative models, to calculate radioactive concentrations in urban areas and surrounding open country, taking account of natural and artificial obstacles in the short field, different architectural layouts, and different local meteorological conditions. The work performed during phase-I is concluded. The modular structure and all models are ready for phase-II, during which the calculation of radioactive concentrations and comparisons with other codes for validation purposes will be carried out. Phase 2 will begin from the first year of the next three-year national plan.

Note

Copia n. **In carico a:**

REV.	DESCRIZIONE	DATA		REDAZIONE	CONVALIDA	APPROVAZIONE
2			NOME			
			FIRMA			
1			NOME			
			FIRMA			
0	EMISSIONE	25/09/15	NOME	F. De Rosa	P. Meloni	F. De Rosa
			FIRMA			

TABLE OF CONTENTS

A. INTRODUCTION

In the Western Countries, mainly after Fukushima accident, there has been a strong need to review the safety margins of plants in operation or under construction and to proceed to a renewed commitment on nuclear safety & security field and on fuel cycle management and waste reduction. In Italy, where with a public poll was decided to stop the use of nuclear power plants to produce electricity, it was not more necessary to perform studies and applications to improve the industrial standard of such systems. Nevertheless, Italy is a technologically advanced country, aligned with the safety standards of other Western countries, therefore an obligation to keep alive the scientific knowledge in the field of nuclear fission, giving priority to the maintenance of knowledge in the safety and security field, remains mandatory.

The new Italian task is to concentrate efforts both in research and in international cooperation for the safe use, even beyond its geographical boundaries, of existing plants and on nuclear power plants of next generation. The new context that emerged in Italy after Fukushima accident and the subsequent referendum, has led to make a review of priorities planned before this worldwide negative event.

One of the most relevant consequences derived by the revision of the national nuclear plan was to proceed towards the preservation of a nucleus of scientific experts in the field of nuclear safety and security and to promote studies for the development of Generation IV systems.

This report describes the activities performed to conclude phase-I. The modular structure and all models are ready for phase II, during which the calculation of radioactive concentrations and comparisons with other codes for validation purposes will be carried out. Phase-II is planned as work for the next three-year PAR national project.

B. SHORT HISTORY

At the moment, three different modules characterize RADCAL code structure. RADCAL is a computational tool, relatively “fast-running”, belonging to the HYDRA Code Package, developed in ENEA to evaluate the external impact of severe accident scenarios occurring in NPPs.

Originally, RADCAL was developed to evaluate the impact of pollutants released on the harbors and surrounding areas in which is foreseen the presence of military units equipped with nuclear propulsion engines. RADCAL-II was used as complementary tool, for comparisons with HOTSPOT code results, to help for the identification of radioactive risk level in order to review the national emergency plan, to be issued as "Technical Report" subject to evaluation by a Committee pursuant to article 9 of D.Lgs.230/95. RADCAL-III is the civil version of RADCAL-II. It is not a trivial

translations of models but a real new structure to evaluate the external consequences of scenarios initiated by a severe accident event.

RADCAL-III structure is designed to take account of two different situations. The first one is studied in the ambit of the EDEN project (End-user driven DEmo for cbrNe[1]), funded by the European Union, in the Seventh Framework Programme (FP7/2007-2013), under the Grant Agreement no. 313077. This research work is aimed at developing and validate models inside RADCAL-III for the evaluation of accidental releases of radiological material to environment as a consequence of the explosion of a dirty bomb. A Thematic Demonstration RN4.2, organized by ENEA, is foreseen at the end of September 2015, and focused on the "Remote monitoring and identification of a dirty bomb containing explosive and radiation materials and on a calculation of external consequences in the case of explosion". The demonstration aims at testing, on the field, innovative technologies for remote detection of a Dirty Bomb and for an estimate of the consequences to environment and people in the case of explosion in critical and or highly populated areas. This part of RADCAL-III structure is called «module R» ("Radiological Module").

The other part of RADCAL-III structure is called «module N» ("Nuclear Module") and represents the object of the present work.

It is worth noting that all models under development refer to the instantaneous release of pollutants (puff mode). This initial statement is necessary to put in evidence that the new mathematical approach adopted is strongly different by that commonly used to describe steady state releases. These new models allow the user to investigate the consequences caused by radioactive pollutants released under transient conditions. The zone of interest is the atmosphere under the planetary boundary layer (PBL) because the event initiates at (practically) ground level and when pollutants are transported far away from the "point-zero" they are so violently dispersed that the effects of impact with PBL are not so significant as in the case of a continuous plume[2]. Puff models under development in RADCAL-III are based on the Eulerian approach.

Further corrections in the short field[3] have been made by using experimental data available from wind gallery experiments, in order to take into due account the presence of atmospheric turbulence and natural or artificial obstacles (mountains, buildings, etc).

In the case of nuclear releases, generally the territory interested may be very large, because the plume generated can be transported by winds at very long distances from the source. RADCAL-III mod. N allows to perform calculations of airborne and ground

[1] The acronym CBRNE stand for "Chemical, Biological, Radiological, Nuclear, and Explosive".
[2] Typical release from chimney stacks at considerable height.
[3] Zone in which the influence of obstacles is not negligible.

concentrations in urban areas and open country at maximum horizontal distances from the source belonging to the meso-alpha subclass[4].

C. DOCUMENT STRUCTURE

In order to describe the most relevant steps relating to mathematical, physical, meteorological and architectural aspects and to show how the code is structured for the preparation of the input deck, this technical report is divided in two parts.

The first is devoted to theory and the second one to GUI (Graphic User Interface) description and to show how data for input deck preparation are inserted.

Both parts are particularly interesting because many examples and explanations will be provided to make as clear as possible the description of the whole work performed during phase-I.

[4] Range 200-2000 km.

PART 1: MATHEMATICAL, PHYSICAL, METEOROLOGICAL AND ARCHITECTURAL ASPECTS

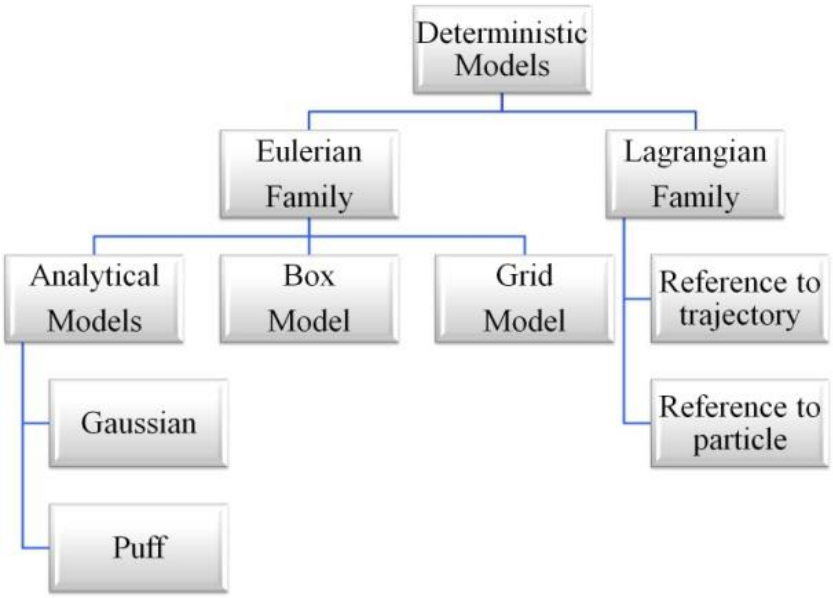
1. MATHEMATICAL MODELS

There are many ways to realize a model and it is not the case here to describe all them. Generally speaking, we can say that there are two fundamental classes of models: deterministic and probabilistic.

What is better for our scope?

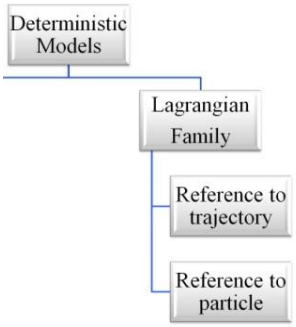
Let us say that deterministic models are based on a strong relation between cause and effect, while the stochastic ones on real measures performed in well identified zones of the territory, mainly those close to industrial plants or in critical urban areas to be taken under cautious control. It is worth noting that probabilistic models can really predict pollutants behavior only in those points in which measures are made, even if later, with proper adjustments and improved algorithms, they are applied also outside their basic dominion of validity.

When the application is not referred to a very specific target, deterministic models are preferred, even though they are never completely free of simplifications, specific limitations and so on.

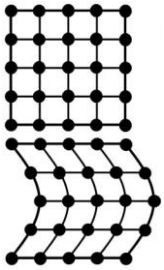


1.1 Lagrangian approach

Lagrangian models make reference to a mobile Cartesian system in order to follow particles mass motion or their trajectories. The Lagrangian family models the motion of the particles as a random walk process. It is characterized by trajectory and particle models.



Trajectory models simulate the evolution of a fluid (air) driven by wind speed (horizontal component).



Particle models simulate pollutants emission step by step evaluating the concentration in function of particles number flowing through a control volume. In this cases, pollutants are not considered as a continuous fluid immersed into another continuous fluid (the carrier gas is atmospheric air).

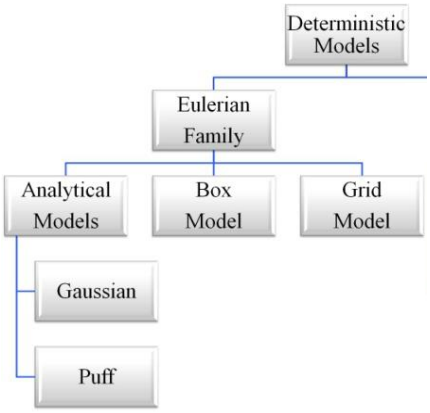
There is a group of independent particles, each one characterized by proper trajectory, immersed into a fluid subject to turbulent fluctuations.

It must be said that the PBL is characterized by turbulent motions (whirls), thus it is not possible to make use of a deterministic approach to well describe the single particle trajectory. Stochastic trajectories and turbulence are clearly difficult aspects to take into account in the motion simulation. It means that a fairly complex approach is necessary to simulate an explosion and its consequences.

The Lagrangian approach is without any doubt a very attracting way to simulate particle motion with good approximation, but in our case the primary purpose is to obtain results as soon as possible, even if affected by slightly higher errors. Our interest, in any case, is to realize models sufficiently reliable and, at the same time, not extremely complex or high CPU time-consuming. This choice is supported by the fact that the uncertainties cannot be eliminated only by the choice of the descriptive model, since they depend on a number of factors independent of each other, such as the user skillness, the operating system, the level of optimization of the data processing structure, the accuracy of the choices made in neglecting or taking into account the various phenomena and still more.

1.2 Eulerian approach

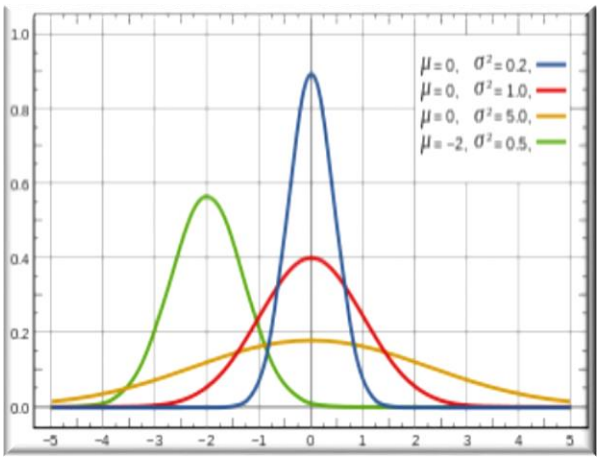
By this approach models are developed under a fully deterministic point of view, describing the motion of a continuous fluid in which another continuous fluid is immersed. The most important difference between Lagrangian and Eulerian approach is that the latter makes use a fixed three-dimensional Cartesian grid as a frame of reference rather than a moving one. Eulerian models are based on the integration of diffusion equation obtained as a mass balance in a control volume.



Depending on the solution adopted, Eulerian approach leads to box, grid or analytical models (gaussian, puff). Box models are called so because the dominion is divided into a certain number of boxes in which air pollutants are perfectly mixed (lumped parameter approach) and estimate the average pollutant concentrations anywhere within the airshed. This approach leads to a quite simple mass balance equation and, knowing wind speed, particle deposition velocity, background concentration, height of mixing boundary layer, the pollutant concentration can be easily calculated. Box models are widely used in air pollution modelling and are simpler than the simulation that can be performed using 3D Eulerian grid models. Grid models, like box ones, divide the dominion into boxes, in which the solution of atmospheric diffusion equation is obtained by finite-difference techniques.

The Eulerian GRID model is based on the realization of a n x n scheme with a large gridsize (many km). Although useful, this approach is not attractive for our purpose because generally the horizontal dimension of boxes is greater than 1 km: too much.

The third group of Eulerian family is the analytical one, characterized by Gaussian and puff models.

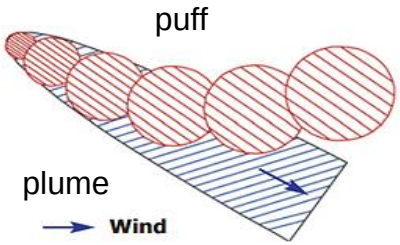


Gaussian model is the most commonly used model type. It assumes that the air pollutant dispersion has a Gaussian distribution, meaning that the pollutant distribution has a normal probability distribution. Gaussian models are most often used for predicting the dispersion of continuous, buoyant air pollution plumes originating from ground-level or elevated sources and evaluate the downstream mass concentration of a pollutant released by a point-source emitting without interruption.

Widely known and largely applied is the gaussian plume model. Conditions for the applicability are: steady state release, homogeneous meteorological situation, only horizontal component of wind speed, no obstacles, no orography, flat ground, no chemical reactions. In addition, they cannot be applied when wind is absent or very wick and for points close to the source.

Puff models are a sort of improved gaussian models and allow to simulate situations under non homogeneous and not steady state conditions and also when the wind is wick or absent.

Mass concentration is calculated as a sum of various puff contributions within a control volume. In this case the following fundamental laws must be respected: momentum and total mass conservation; law of perfect gases; mass conservation of each chemical species acting as pollutant in the carrier gas (atmospheric air).



For cases involving a high degree of spatial variability of the flow within the boundary layer, the assumption of a steady state (Gaussian plume model) may not be valid beyond a few kilometers, and a puff model may be more appropriate to describe the situation.

2. DETERMINATION OF THE MOST SUITABLE APPROACH

To individuate the most appropriate model for our purpose, some fundamental aspects must be evaluated:

a) Spatial scale
b) Time scale
c) Turbulence and meteorology conditions
d) Orography and urban areas
e) Source geometry
f) Information on radioisotopes
g) Release regime

2.1 Spatial scale

In general, mesoscale mainly refers to meteorology, but this terminology can also be applied to horizontal distances from the source.

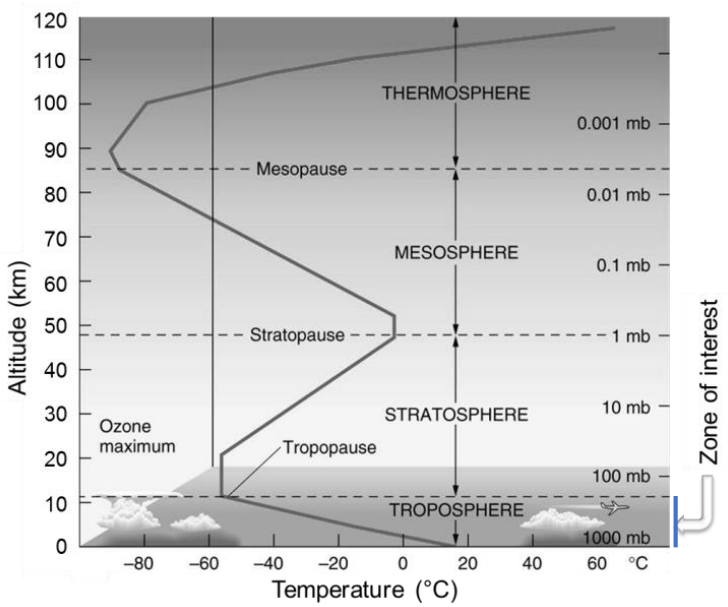
Mesoscale is characterized by three ranges of distances:

- Meso-gamma, from 2 to 20 km;
- Meso-beta, from 20 to 200 km;
- Meso-alpha, from 200 to 2000 km.

RADCAL-III mod. N has been realized with the purpose to investigate releases up to 1000 km from the source, therefore it refers to the meso-alpha dominion.

Concerning the altitude, the zone of our interest is focused on the first layers of the atmosphere and therefore within altitudes not beyond those of the troposphere. In the figure below, the red line shows the variation of the temperature as a function of the

distance from ground level. It can be seen that within the troposphere the temperature decreases when altitude increases.



2.2 Time scale

Short and long term periods are differently treated. Short term is for the evaluation of the plume arrival over the urban area (still transient conditions) while long term models are used to study cumulative expositions and steady state.

2.3 Turbulence and meteorology

The most relevant phenomena influencing pollutants behaviour are wind and turbulence. Only in few cases the parameters describing these phenomena can be considered homogeneous and subject to steady state conditions. Wind speed and direction are dependent on orography and on local processes, while turbulent diffusion is function of mechanical and convective characteristics of the zone under investigation.

Turbulence, with formation of whirls, may arise when a fluid is locally perturbed by external actions sufficiently intense to create local velocity and high velocity gradients. According to (stochastic) theory formulated by Kolmogorov in 1941, a hierarchy of whirlwinds of increasing size, interconnected to each other, must be considered.

Each spheroidal whirl, has an own rotational-translational motion and disappears generating a smaller secondary whirl. Whirls of greater size have an asymmetrical spheroidal shape, while those smaller become more and more comparable to spheres and their rotational speed increases. The energy supplied to the fluid can be seen as

a sort of “energy cascade”. We can consider that, among larger vortices, the energy transfer occurs without dissipation (slow rotation), but when smaller whirls are involved, energy is dissipated in the form of heat, due to their high rotation speed and the interaction (friction) with the surrounding fluid.

According to Kolmogorov’s hypothesis, the energy dissipation rate for smaller whirls is equal to the rate of energy acquired by whirl earlier in the hierarchy (steady-state condition).

Omitting some steps, we can write:

$$\vartheta_k = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \qquad \upsilon_k = (\nu * \varepsilon)^{1/4} \qquad \tau_k = \left(\frac{\nu}{\varepsilon}\right)^{1/2} \qquad /1/$$

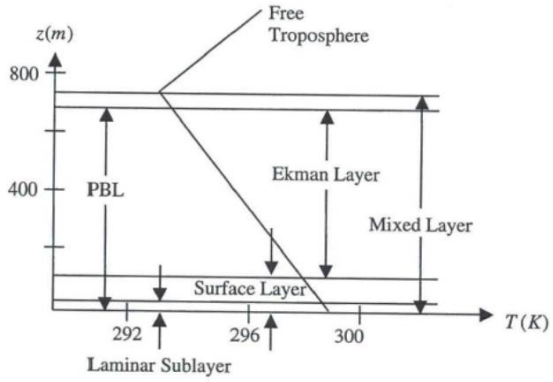
where (*k stands for Kolmogorov*):

- ϑ_k= mean diameter of whirl (cm)
- $\nu = \text{kinematic viscosity} = \frac{\eta}{\rho}$

  $\eta = \text{dynamic viscosity}, \rho = \text{fluid density}, \varepsilon = \text{input/dissipation energy rate}$[5].
- $\upsilon_k = \text{average rotational speed},$
- $\tau_k = \text{mean lifetime}$

We can see that when ε increases:

- The dimension of the last whirl (the smallest) of hierarchy decreases;
- The average rotational speed of smallest whirl increases;
- The lifetime of smallest whirl decreases.



It means that a strong local perturbation can generate very small whirls, with high rotational speed far from the perturbation itself. These small whirls have a lifetime shorter than larger whirls located near the origin of such a perturbation. As previously written, troposphere is the dominion in which our interest is concentrated and 2000 m is the maximum altitude to be considered, since we want to study the effects caused by the dispersion of material released practically at ground level.

It means that we can concentrate our attention up to mesoscale (local transport of pollutants) within the Planetary Boundary Layer (PBL), that is the part of the atmosphere, who extends between 1 and 2 km above the ground level, within which the motion of the fluid is influenced by the conditions of the surface below. The vertical

[5] Is the heat produced by energy dissipation per unit of mass and time.

length, between ground and extreme PBL boundary, is called *mixing height*. The altitude at which we have the first temperature inversion is approximately equal to the limit of the PBL. Normally, the air near the Earth surface is warmer than the air above because solar radiation warms the Earth surface, which in turn warms the layer of the atmosphere directly above it. Thus, the atmospheric temperature normally decreases with increasing altitude. However, under certain meteorological conditions, in some atmospheric layers (called inversion layers) temperature may increase with increasing altitude. Inversion layers, formed at some distance above ground level, can act as a lid for the air below. Thus, any air pollution plume that enters an inversion layer will undergo very little vertical mixing unless it has sufficient momentum to completely pass through.

When an inversion layer is formed at a certain altitude above the Earth, the atmospheric layer between the Earth surface and the bottom of the inversion layer is known as mixing layer and the distance between the Earth surface and the bottom of inversion layer is known as mixing height.

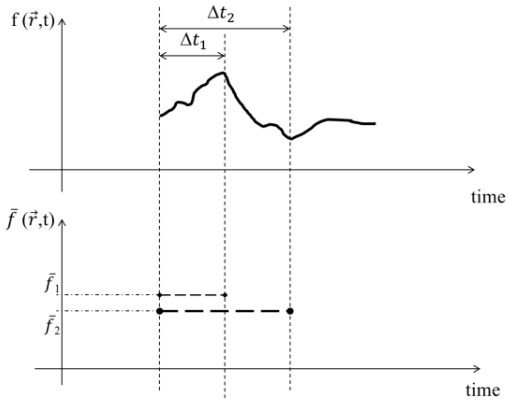
Even if a pollution plume penetrates the inversion layer, it will not undertake any further significant vertical mixing. The knowledge of mixing height becomes very important to well simulate the evolution of air pollutant plume.

When pollutants are released inside a turbulent fluid (air), they are strongly dispersed by roto-translational motion of the whirls. Although the velocity field $\bar{u}\,(\bar{r}, t)$ is fully described by Navier-Stokes equations, the numerical solution is not possible when the regime is turbulent.

To take correct account of the smaller whirls, it should be necessary to discretize the space into very small cells and take very short time intervals. A correct description of the phenomena is strongly linked to the accurate description of smaller whirls.

Only with the intent to anticipate some concepts of the more detailed treatment that will be made below, let say something about turbulent diffusion coefficients.

Let us introduce the concept of temporal average (at each point $\bar{r}$) of a generic function f ($\bar{r}$, t) considering a time window of width Δt, extended from t-Δt/2 to t+Δt/2.



It is clear that the mean value of the function f ($\bar{r}$, t) will depend on the width of Δt.

We can write:

$$\bar{f}\,(\vec{r}, t) = \frac{1}{\Delta t} \int_{-\Delta t/2}^{\Delta t/2} f(\vec{r}, t+\tau)\, d\tau \qquad /2/$$

Applying eqn. /2/ to wind speed $\bar{u}$ and to pollutant concentration $\bar{C}$:

$$\bar{u}\,(\vec{r},t) = \frac{1}{\Delta t}\int_{-\Delta t/2}^{\Delta t/2} u(\vec{r},t+\tau)\,d\tau$$

$$\bar{C}\,(\vec{r},t) = \frac{1}{\Delta t}\int_{-\Delta t/2}^{\Delta t/2} C(\vec{r},t+\tau)\,d\tau$$

After some omitted mathematical steps, we can write:

$$\frac{\partial \bar{C}(\vec{r},t)}{\partial t} = -\nabla\left[\bar{u}(\vec{r},t)\,\bar{C}(\vec{r},t)\right] - \nabla\left\langle u_f(\vec{r},t)\,C_f(\vec{r},t)\right\rangle_{\Delta t} \qquad /3/$$

where:

- $\bar{C}(\vec{r},t) = mean\ air\ pollutant\ concentration.$
- $\bar{u}(\vec{r},t) = mean\ wind\ velocity.$
- $C_f(\vec{r},t) =\ concentration\ difference\ between\ the\ true\ concentration\ value\ at\ time\ t\ and\ average\ value, C_f(\vec{r},t) = C(\vec{r},t) - \bar{C}(\vec{r},t)$
- $u_f(\vec{r},t) =\ velocity\ difference\ between\ the\ true\ velocity\ value\ at\ time\ t\ and\ average\ value, u_f(\vec{r},t) = u(\vec{r},t) - \bar{u}(\vec{r},t)$

It is now necessary to develop a model to process the term $\left\langle u_f(\vec{r},t)\,C_f(\vec{r},t)\right\rangle_{\Delta t}$ bearing in mind that we need a "*closure relation*", because any possible assumption goes beyond fluid dynamics concepts.

The basic theory developed by Boussinesk in 1877, called "*Gradient Transport Theory*" or "*First-Order Closure*", can be very useful.

We report here only the conclusive relations, omitting intermediate steps.

It is possible to write:

$$\begin{cases} \left\langle u_{x,f}(\vec{r},t)\,C_f(\vec{r},t)\right\rangle_{\Delta t} = -D_{w,x}(\vec{r},t)\,\dfrac{\partial \bar{C}(\vec{r},t)}{\partial x} \\ \left\langle u_{y,f}(\vec{r},t)\,C_f(\vec{r},t)\right\rangle_{\Delta t} = -D_{w,y}(\vec{r},t)\,\dfrac{\partial \bar{C}(\vec{r},t)}{\partial y} \\ \left\langle u_{z,f}(\vec{r},t)\,C_f(\vec{r},t)\right\rangle_{\Delta t} = -D_{w,z}(\vec{r},t)\,\dfrac{\partial \bar{C}(\vec{r},t)}{\partial z} \end{cases} \qquad /4/$$

Where:

$D_{w,x}(\vec{r},t), D_{w,y}(\vec{r},t), D_{w,z}(\vec{r},t), are\ the\ turbulent\ diffusion\ coefficients\ in\ x, y\ and\ z\ directions.$

Substituting /4/ in /3/:

$$\frac{\partial \bar{C}(\vec{r},t)}{\partial t} = \underbrace{-\nabla\left[\bar{u}(\vec{r},t)\,\bar{C}(\vec{r},t)\right]}_{\text{advection due to mean flow}} + \underbrace{\nabla\, D_w(\vec{r},t)\,\nabla\,\bar{C}(\vec{r},t)}_{\text{turbulent diffusion}} \qquad /5/$$

To be accurate, we should not speak of turbulent diffusion, but of molecular dispersion for the presence of chaotic whirls vortices chaotic able to produce turbulence inside an originally laminar flow.

2.4 Orography and urban areas

Only in few cases the territory can be classified flat ground. In many cases we need to perform simulations in complex urban areas, where a lot of obstacles are present (artificial and natural) or in open country, over which pollutants dispersion can also be influenced by the history of plume, “lived” during its passage in zone where interferences to dispersion are present.

When cases such as the release of radioactive pollutants by NPPs are studied, a complex combination of areas must be taken into account. Not to be excluded is the co-presence of sea and soil, urban and country areas, densely populated areas followed by industrial plants, and so on. This is only one of the possible cases, therefore is not completely correct evaluate the situation in atmosphere and at groun level with a too-much simplified tool. It is necessary to take account of obstacles, canyons, city layout, wind speeds, local meteorological conditions, humidity, vertical gradients, deposition, radioactive decay and so on.

2.5 Source geometry

To study pollution due to urban traffic, linear sources simulating roads should be used. Pollution by industrial plants require investigations of emissions from a stack (single point-source) or chimney stacks (multiple point-sources). A point source has no geometric dimensions.

To maintain under continuous control large urban areas or countryside, an areal or a volumetric source should be modeled. An area source is a two-dimensional source of diffuse air pollutant emissions. A volume source is a three-dimensional source of air pollutant emissions. Essentially, it is an area source with a third (height) dimension.

In our case is sufficient to consider a point-source emitting several pollutants instantaneously (like a puff) and a successive plume expansion all along the area of interest.

2.6 Information on radioisotopes

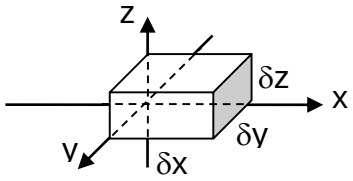
We can have one or more gases, aerosols and particulates with different size and shape. In our case the released material is radioactive. Pollutants can remain airborne for long time or be characterized by proper deposition velocity. Humid and dry deposition processes may be taken into account or not, and so on. In our case it is very important to get as many information as possible regarding the airborne and the ground material concentration in short field, and dispersion level (mainly) of gases in far field. It means that two different models must be used, one suitable for short field and the other one for far field (still urban or already open country).

2.7 Release regime

To study the effects of emissions from chimneys or traffic pollution, steady state regimes can be considered. In all other cases and mainly when the evolution is time-dependent (as in our case), these models cannot be used. All that said, we can conclude that puff release models are the most attractive for our scope, but they are not good enough to well describe a variety of situations and configurations of our interest. So, our choice is the adoption of puff models but a series of changes, corrections and improvements will be made in order to satisfy at best our real and different situations.

3. BASIC GAUSSIAN PUFF MODEL

To write the general equation for the concentration of the i-th pollutant, let us consider a control volume Vc with dimensions δx, δy, δz as shown in figure.



The speed of a generic pollutant flowing through volume Vc is given by:
$\vec{u} \equiv (u_x, u_y, u_z)$ so that the time derivative of concentration for the i-th pollutant is:

$$\frac{\partial C_i}{\partial t}\,\delta x\,\delta y\,\delta z = -\left[\frac{\partial (C\,u_x)_i}{\partial x} + \frac{\partial (C\,u_y)_i}{\partial y} + \frac{\partial (C\,u_z)_i}{\partial z}\right]\delta x\,\delta y\,\delta z + (S_i + R_i + \mathrm{K}_i)\,\delta x\,\delta y\,\delta z$$

$$\frac{\partial C_i}{\partial t} = -\frac{\partial (C\,u_x)_i}{\partial x} - \frac{\partial (C\,u_y)_i}{\partial y} - \frac{\partial (C\,u_z)_i}{\partial z} + S_i + R_i + \mathrm{K}_i \qquad /6/$$

Where:

- $\frac{\partial C_i}{\partial t}$ = time-derivative of the i-th pollutant concentration in Vc.
- $\frac{\partial (C\, u_x)_i}{\partial x}, \frac{\partial (C\, u_y)_i}{\partial y}, \frac{\partial (C\, u_z)_i}{\partial z}$ = derivatives of flow through δx, δy and δz.
- S_i = Source of the i-th pollutant entering Vc
- R_i = Removal term for loss of the i-th pollutant in Vc
- K_i = Removal term for chemical interaction of i-th pollutant with another pollutant.

Eqn. /6/, as shown, cannot be solved (even if the system is closed) because there are instantaneous variables in presence of turbulence in PBL. Turbulent motions are generally characterized by whirls, that can be greater or lesser than puff dimensions. In the first case the whirl incorporates the puff or, at least, puff changes its trajectory. In the second case the puff incorporates the whirl changing its dynamic status and density.

In real situations both cases occur at the same time, thus the global process becomes more and more difficult to simulate. A method to change instantaneous variables into mean values is requested.

It must be noted that in general:

- All variables needed to define the time-space evolution of PBL are stochastic.
- Space-time variation can be defined through a limited number of central moments.
- Mean values are identified as time-average parameters.

To calculate pollutants concentration, time by time, as already made we can refer to Reynolds hypothesis:

$$C_i = \bar{C}_i + C_{fi} \qquad /7/$$

Where:

- $C_i = instantaneous\ concentration\ of\ the\ i-th\ pollutant.$
- $\bar{C}_i = mean\ concentration\ of\ the\ i-th\ pollutant.$
- $C_{fi} = difference\ between\ the\ true\ concentration\ and\ average\ concentration\ of\ the\ i-th\ pollutant.$

Applying Reynolds hypothesis to all conservation equations, we obtain “mean value” equations, but in some of them second order moments cannot be neglected (variances and co-variances). This is the specific case of momentum equation.

Substituting /7/ in /6/:

$$\frac{\partial \bar{C}_i}{\partial t} = -\left(\bar{u}_x \frac{\partial \bar{C}_i}{\partial x} + \bar{u}_y \frac{\partial \bar{C}_i}{\partial y} + \bar{u}_z \frac{\partial \bar{C}_i}{\partial z}\right) + \left(\frac{\partial \left(\overline{u_{fx}\, C_{fi}}\right)}{\partial x} + \frac{\partial \left(\overline{u_{fy}\, C_{fi}}\right)}{\partial y} + \frac{\partial \left(\overline{u_{fz}\, C_{fi}}\right)}{\partial z}\right) +$$

$$+ \bar{S}_i + R_i + K_i \qquad /8/$$

To slightly simplify eqn. /8/, K_i can be considered negligible because we have assumed that pollutants of one kind do not react with pollutants of other species. The removal term R_i represents the loss of pollutants, mainly by radioactive decay and secondarily by gravitational settling. This term can be temporarily omitted. It will be taken into due account later. S_i is the mass of i-th pollutant entering Vc and depends only on its chemical characteristics and on the type of release. The time-spatial evolution of the "i" equations shown in /8/ depends directly on meteorological conditions due to the presence of the mean wind speed.

The system of equations /8/ is not closed because the number of variables is not the same of number of equations, therefore a closure is required.

A first consideration is that, even though adopting a corrective approach, the system of fluid-dynamic equations describing a turbulent status of PBL can never be directly solved or closed. Nevertheless, it does not mean that a solution is impossible.

To solve the problem (applying a closure) we will handle only equations with mean variables, taking care to approximate the other ones (unknown variables representing moments of higher order) with semi-empirical relations based on experience or derived from results obtained by using experimental facilities.

Two types of closure are possible:

- General;
- Local.

The general closure is based on the concept that all turbulent whirls transport a certain amount of fluid only for limited distances. In this case, advection is assumed as the governing process, while when local closure is used, the governing process is diffusion (assimilable to molecular diffusion).

In our case a local closure is more appropriate.

The most adopted is the "k-closure", who permits the use of local gradients of mean variable instead of turbulent flows (similar approach followed to obtain eqns. /4/):

$$\begin{cases} \overline{u_{fx}\, C_{fi}} = -K_{xx}\, \dfrac{\partial \bar{C}_i}{\partial x} \\ \overline{u_{fy}\, C_{fi}} = -K_{yy}\, \dfrac{\partial \bar{C}_i}{\partial y} \\ \overline{u_{fz}\, C_{fi}} = -K_{zz}\, \dfrac{\partial \bar{C}_i}{\partial z} \end{cases} \qquad /9/$$

Substituting /9/ in /8/:

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}_x \frac{\partial \bar{c}_i}{\partial x} + \bar{u}_y \frac{\partial \bar{c}_i}{\partial y} + \bar{u}_z \frac{\partial \bar{c}_i}{\partial z} = -\left[\frac{\partial}{\partial x}\left(K_{xx} \frac{\partial \bar{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy} \frac{\partial \bar{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz} \frac{\partial \bar{c}_i}{\partial z}\right)\right] + \bar{S}_i \quad /10/$$

Where:

K_{xx}, K_{yy}, K_{zz}= turbulent diffusivity coefficients.

Eqn. /10/ is the formulation of semi-empirical Eulerian equation to evaluate the concentration of an i-th air pollutant and has been obtained according to the following conditions and simplifications:

- *Adoption of k-closure*, in which is implicitly assumed that mass flow through x, y and z is independent. This should be considered a model weakness, especially when convective flows cannot be neglected.
- *Meteorological model de-coupling*. Practically, is the de-coupling of mass balance equations for all "i" pollutants, in which the evolution of meteorological mean variables is described.
- *Parameterization of turbulent diffusivity coefficients*. It is assumed that atmospheric turbulence depends only on diffusivity coefficients Kxx, Kyy, Kzz.

Generally, eqn. /10/ does not allow analytical solutions, due to assumptions above and to the fact that a mean wind field is taken into account.

In any case, considering that:

- Our models should describe an instantaneous release of a certain number of pollutants, whose main impact is more relevant than the impact of potential secondary particles created by chemical interactions with other pollutants.
- Wind meteorology in open country is important, but in our case it is not the most relevant variable influencing the behaviour of pollutants all along their trajectories, especially in short field, where generic obstacles, buildings, canyons and many other overhangs are present.
- Turbulence is absolutely important, but in short field and at ground level or, in any case, at levels not higher than 50 meters, also other variables, such as wind direction and the percentage of area occupied by obstacles (buildings,…) can deeply interfere with pollutants trajectories.

An analytical solution of eqn. /10/ is possible provided that the following conditions are respected:

- The source of pollutants is centered in the origin of an orthogonal Cartesian system

  ➔ O ≡ $(0,0,0)$.
- The x-axis is oriented to the wind direction.
- At time t = 0 an instantaneous puff of pollutants is released by source.
- Wind field is uniform both in horizontal and vertical directions and its speed value is u.
- Turbulent diffusivity coefficients Kxx, Kyy, Kzz are constant.

This way, we can write that the concentration C_i in a generic point $P_i \equiv (x_i, y_i, z_i)$ at time t of an i-th pollutant released with initial mass m_i by a punctiform source is given by:

$$C_i(x,y,z,t) = \frac{m_i}{(4\pi t)^{3/2}\left(K_{xx}K_{yy}K_{zz}\right)^{1/2}}\, e^{-\frac{1}{4t}\left[\frac{(x-ut)^2}{K_{xx}}+\frac{y^2}{K_{yy}}+\frac{z^2}{K_{zz}}\right]} \qquad /11/$$

Comparing eqn. /11/ to the general formulation of gaussian function:

$$F(x) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\left[\frac{(x-x_m)^2}{2\sigma^2}\right]} \qquad /12/$$

we can note a very tight correspondence.

Indeed eqn. /11/ is known as "*basic gaussian puff model*", derived from the semi-empirical Eulerian formulation. A model based on assumptions made to write eqn. /11/, but properly adjusted to take into account a series of variables relevant to describe the situation that we want to simulate, can now be constructed.

4. CORRECTIONS WITH THE USE OF EXPERIMENTAL DATA

In previous chapters, we have seen that using conservation equations and making successive simplifications, it is possible to obtain analytical solutions for the problem of our interest, that is the description of pollutants in PBL as a consequence of a sudden release, due to an explosive event at a NPP. We have also seen that to find analytical solutions, whatever approach is selected, a certain number of assumptions, corrections and simplifications is necessary.

A logical consequence is that, in any case, the results are burden with a non negligible level of uncertainty. On the other hand, we can say that all approaches are not perfect, each one suffers from own weaknesses, therefore our selected model, even if constructed after a series of assumptions heavily idealized, is attractive because simple and easy to manage.

Nevertheless, to make a gaussian-based model sufficiently valid for our scope, a certain number of additional corrections must be inserted in eqn. /11/. Under this point of view, a valid help comes from data and results obtained by experiments performed at the wind gallery. The need of experimental data to make all due corrections to theoretical models, leads to the realization of empirical and semi-empirical models. In some cases, from the mathematical and physical point of view, this approach is not widely accepted. Theorists and purists prefer a fully rigorous approach, but it won't always be possible.

An example could help to understand why.

We have seen that after some corrections and assumptions, a basic gaussian puff model, derived from the semi-empirical Eulerian formulation, has been obtained. In a similar manner, also Lagrangian relations can lead to a basic puff model, even though by this way a final closure is not needed. So analogous puff models can be realized using both the Eulerian and the Lagrangian approach.

At this point, a reasonable question arises: "Can the two basic puff models, independently derived by Lagrangian and Eulerian approaches, be considered equivalent?"

Provided that both methods have rigorously been applied, the answer should be: "Yes", but let us make a deeper look to verify if this answer is really right.

Omitting all steps necessary to get both formulations, easily findable in open literature, we report here only the final relations useful to perform the comparison.
Let us consider the vertical dispersion of a pollutant in a volume characterized by homogeneous turbulence and stable conditions. It means that fluid properties, either deterministic or stochastic, remain unchanged at all time. It follows that $\sigma_{w_{fluid}}$ and $\sigma_{w_{pollutant}}$ are constant. In addition, also the turbulent diffusivity coefficient K_{zz} does not change because, by definition, it is a property only of fluid motion.

Adopting the Lagrangian approach (no closure needed), we have:

$$\frac{d\sigma_z^2}{dt} = 2\,\sigma_w^2 \int_0^t R(\tau)d\tau \qquad /13/$$

Where:

- σ_w^2 = Variance of particle vertical speed. It gives the mean temporal irregularity of particle velocity during motion.
- τ = Time lag. It is the time elapsed between two successive values of stochastic variable.
- $R(\tau)$ = Coefficient of Lagrangian autocorrelation. It gives the correlation between particle velocities in two different instants separated by the time interval τ. This parameter is a sort of measure of what percentage of particle velocity at time t is "*remembered*" at time t+τ.

Eqn. /13/ gives two different solutions, the first is valid in short field (near the source), the second one in far field:

$\sigma_z^2 = \sigma_w^2\, t$ ➔ short field

$\sigma_z^2 = \sigma_w^2\, T_L\, t$ ➔ far field

- T_L = Decorrelation time. It represents the time necessary to particle, measured from pollutant emission, to "*forget*" its initial velocity value.

Moving now to the Eulerian approach, it is important to remember that the type of closure influences the final formulation.

Going ahead with k-closure, we find:

$$\frac{d\sigma_z^2}{dt} = 2\,K_{zz} \qquad /14/$$

Considering an emission at level z=0, at time t=0 and with null horizontal transport (u=0), the solution is:

$$\sigma_z^2 = 2\,K_{zz}\,t$$

If we want that eqn. /13/ and /14/ give equivalent results, it is necessary that:

$$K_{zz} = \sigma_w^2 \int_0^t R(\tau)d\tau \qquad /15/$$

Unfortunately, relation /15/ is paradoxal. In fact, by definition, in Eulerian approach K_{zz} is constant because referred to a homogeneous fluid while here (see the right hand member) it depends on the time from the initial pollutant release. In order to find when K_{zz} can be considered time-independent, that is when the particle "*forgets* " its history, let us analyze relation /15/ considering that a good approximation for Lagrangian autocorrelation is given by: $R(\tau) = e^{-\tau/T_L}$.

Omitting some simple steps, we obtain:

$K_{zz} = \frac{\sigma_w^2}{T_L}\left(1 - e^{-\tau/T_L}\right)$ /16/

T_L, once pollutant and fluid status are identified, is constant thus, in order for K_{zz} to become (practically) time-independent, it is necessary that $(1 - e^{-\tau/T_L}) \geq 0.99$.

This condition is obtained when $e^{-\tau/T_L} \leq 0.01$, that is when $\tau \geq 4.61\, T_L$.

If, for instance, T_L = 200 s, K_{zz} becomes time-independent only when $\tau \geq 922\ s$.

It means that if we have a wind speed u = 2 m/s, Kzz is time independent only at a distance of about 1800 m from the source.

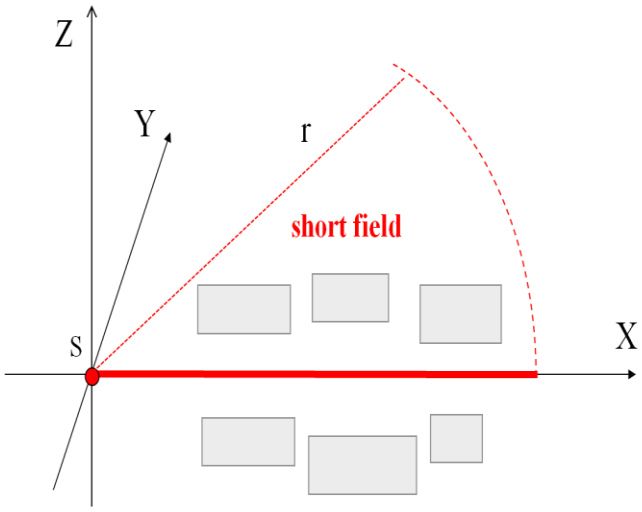
For shorter distances K_{zz} cannot be considered time independent and this is the announced paradox. The conclusion is that a basic gaussian puff model, obtained with k-closure from the semi-empirical Eulerian formulation, is not suitable to describe the behavior of pollutants in short field.

How much more the pollutant is far from the source, the less is the difference between Lagrangian and Eulerian approaches.

From now on, we need to find the necessary number of correlations to apply to the basic gaussian puff model elaborated from the semi-empirical Eulerian formulation, in order to be sure that calculated results are reliable both in short and far field.

Last but really not least, another step to perform is the development of an algorithm able to ensure congruence in the border between short and far field. In other words, it is necessary to create a mathematical “seam” so that all values calculated at the end of short field are congruently linked to those at the beginning of far field.

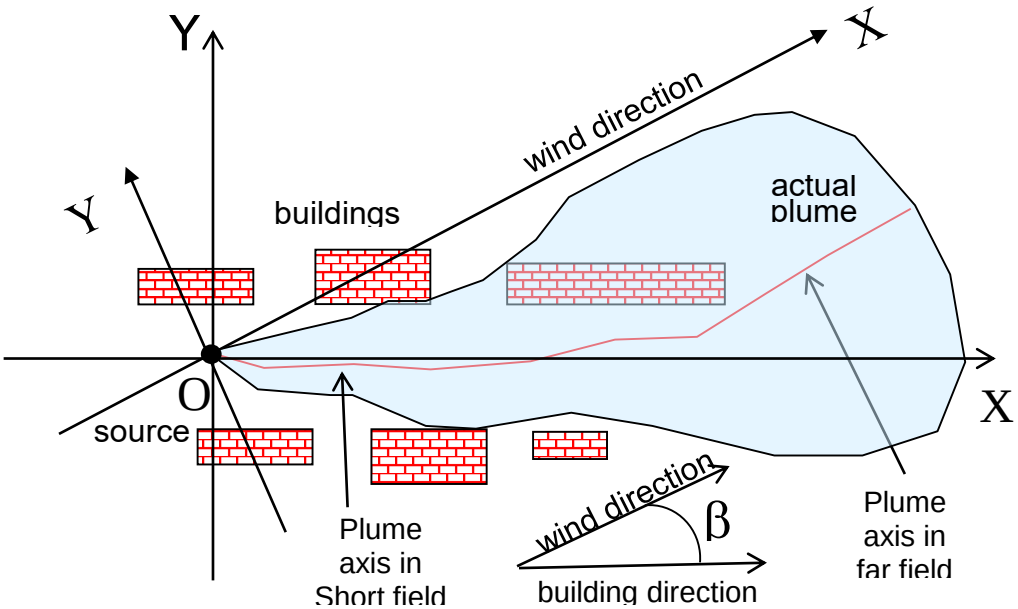
5. SHORT FIELD CONFIGURATION



A circular zone with radius r, all around the source of release, who is centered in the origin, is commonly indicated as short field. The circumference with radius r is the end of short field and the beginning of large field, as shown in figure below.

Apart from very limited cases, in which the accident happens at considerable altitude, natural and artificial obstacles placed in short field can significantly influence the pollutants behaviour.

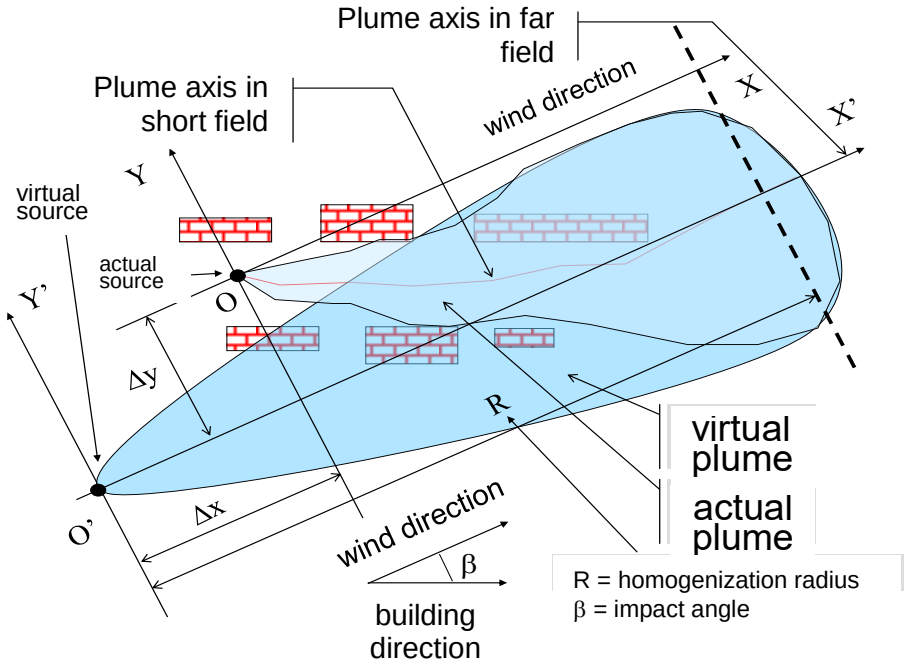
Wind direction becomes a very important parameter. Depending on it, pollutants can pass through obstacles with minimal impact or meet a great obstacle, impossible to cross over. Wind direction forms an angle with x-axis, called impact angle β. In theory β can vary from 0 to $\pi/2$, but for real cases angles between 0 and $\pi/3$ are sufficiently representative of all possible accident events. Angles greater than $\pi/3$ are clearly possible, but in this cases it is better to move x-axis toward a more appropriate direction. It is clear that this situation leads to analyze areas different from those of our original plan. In other words, this is a completely different situation, thus $\pi/3$ represents the real wind direction limit. Once different pollutants are instantaneously released, they are transported by wind and, at the same time, diffused, dispersed, settled, depending on the pollutants nature, size and shape. A plume of pollutants driven by air (in wind direction) is created. If the pollutant is a noncondensable gas, it will be dispersed and diffused all around, increasing its volume and rising. If it is an aerosol, a certain mass remains airborne and transported while the residual is gravitationally settled. As said, settling velocity depends on pollutant nature and particles size and shape. If it is a powder its behavior strongly depends on particles size. If it is a light particulate (~0.1÷2.5 μ), almost all mass can be carried by air for long time. If it has a medium size (2.5÷10 μ) part is transported and part deposited. If it has a large-size (> 10 μ) the mass deposited may prevail respect to that airborne. In any case plume size, shape and dimensions are not easily delineable. A real plume can be schematically drawn as shown in figure below.



Another very important parameter is the space between obstacles. If the space is wide, pollutants can pass through better than where it is narrow. Technically speaking, such space is called “canyon” and we can encounter small, medium and large canyons between obstacles. This concept is very easy to understand when the obstacle is a building and the canyon is the space between two buildings. As we can see in figure above, the plume axis is not a straight line, due to the presence of obstacles and to the fact that, at least during an initial time interval, pollutants in the plume can crash into obstacles and change route and direction. In order to simplify the model, we can consider (even if roughly) a plume axis valid in short field and another one for far field.

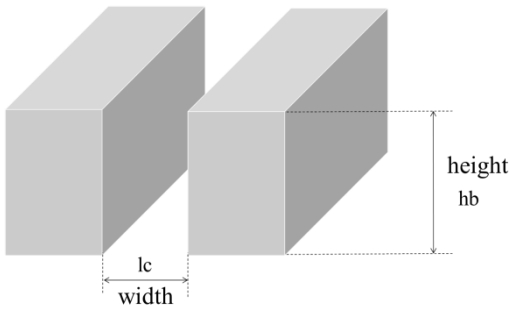
We can also see that in short field plume direction results as a combination of effects between obstacles layout and wind direction and speed, while in far field, when pollutants in the plume are more dispersed and at higher distance from groun level, plume direction is practically governed by wind direction. What said can be schematically represented as shown in figure below, where also the new concepts of virtual plume and virtual source point of application are indicated.

The virtual plume is simply obtained prolonging the x-axis in far field, remaining parallel to the axis of wind direction. To proceed by this way, a new origin point for source must be found. As we can see, referring to Cartesian coordinates of wind, it is located at a certain distance from the real source (where the accident really happens). The real source point has coordinates O $\equiv (0,0,0)$ while the virtual one is O’ $\equiv (\Delta x, \Delta y, 0)$. Δx and Δy will be calculated later on. Following this approach, the concentration of all pollutants can be easily calculated both in short and far field. Wind gallery data can provide these corrective factors, avoiding so to insert additional uncertainties using only analytical models.



5.1 Canyons and obstacles

In short field, where the plume is not much high with respect to ground level, a relevant role is played by canyons and obstacles. Making reference to buildings (but the extension to other types of obstacles is possible) let us have a look at their vertical size, profile and "*ground occupancy*".



It's time to introduce a series of parameters useful to take into account the presence of obstacles.

The first one is known as "*artificial canalization index*" η_c, given by:

$$\eta_c = l_c/h_b \qquad /17/$$

where:
l_c = distance between two buildings (m)
h_b = building height (m)

The *artificial canalization index* provides information about canyon dimensions (width and height) created by the presence of two buildings (obstacles in general).

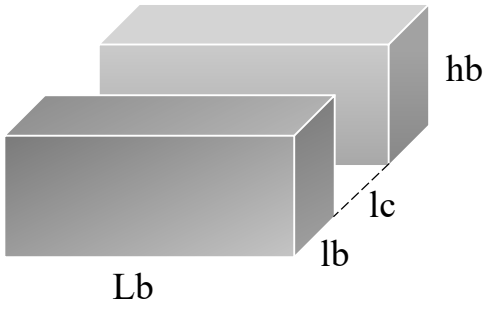
A second parameter is the "*alignment index*", η_a.

It is given by:

$$\eta_a = L_b / l_b \qquad /18/$$

where:

L_b = building length (m)
l_b = building width (m)



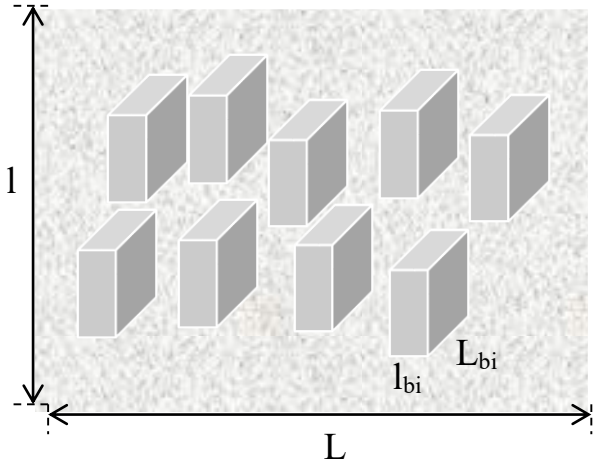
Let us continue introducing now the "occupancy index" η_o, given by:

$$\eta_o = A_{btot} / A_t \qquad /19/$$

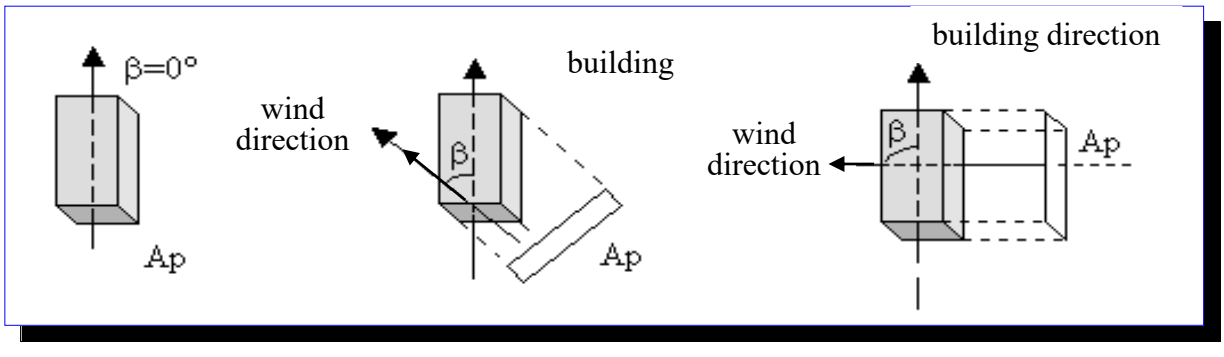
Where:

A_{btot} = Total area occupied by buildings
➔ $A_{btot} = \sum_{i=1}^{n} (L_{b\,i} * l_{b_i})$, in m².

A_t = Total area under investigation
➔ $A_t = L * l$, in m².

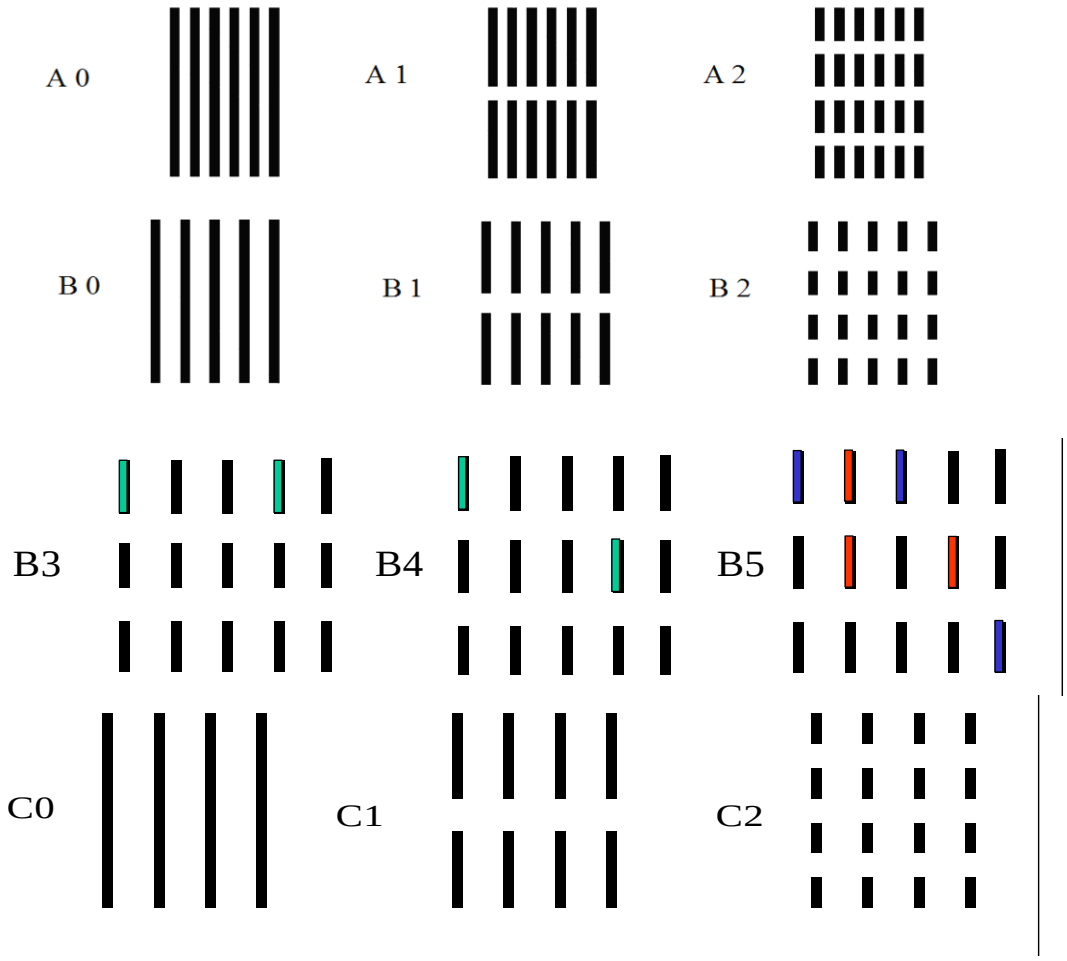


The occupancy index represents the percentage of total area occupied by buildings. Another parameter, not so easy to understand but absolutely necessary for a good simulation, is the "*profile area*", A_p, given by the total obstacle area "seen" by wind direction. In figure below three characteristic situations are shown. The figure in the left represents a situation in which the impact angle is β = 0, that is when wind completely sees the front of building. The figure in the middle is the most difficult to calculate, because represents the total area seen when the impact angle ranges between 0 and $\pi/2$ (0< β <$\pi/2$). The figure in the right shows when β = $\pi/2$ and A_p is the area perpendicular to the main building axis.



We said that in real cases β ranges between 0 and $\pi/3$, therefore A_p can be the frontal building area ($\beta = 0$) or the sum of frontal and lateral areas seen by wind direction ($0 < \beta \leq \pi/3$).

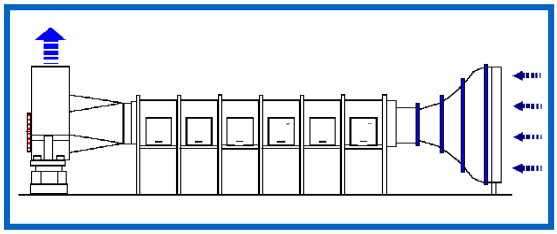
Moving now to canyons, that is the space available for pollutants to pass through obstacles, we have three different types: small (A), medium (B) and large canyons (C).



In the schematic draw above the mean obstacle height is the same, except for configurations B3 ÷ B5, in which obstacles with different height are placed in different positions.

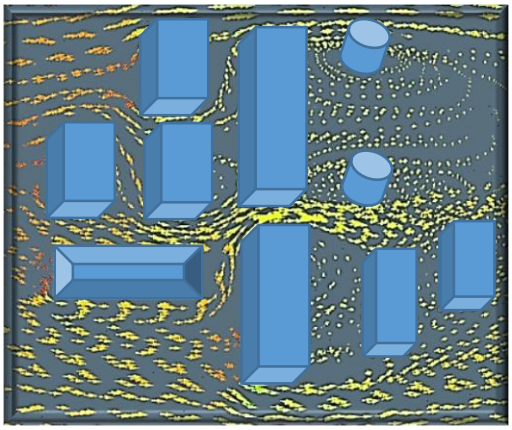
The different layouts shown above can be useful to prepare specific configuration to test in wind gallery, in order to collect information concerning the impact and the pollutants dispersion, even though in scaled dimensions. We know that the "*scaling-factor*" is another important aspect concerning results and databases prepared using data from experiments in lab-scale.

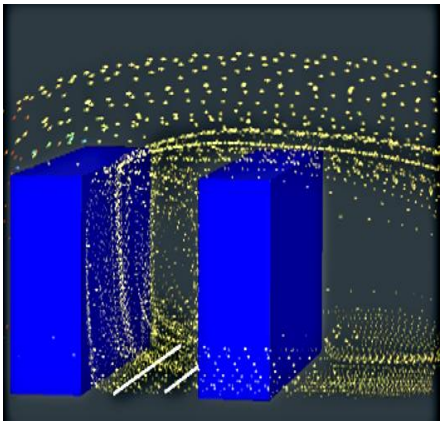
In the two figures below some details of tests conducted at the wind tunnel of Karlsruhe University by Theurer, Plate (1996) using different architectural models, obstacles and canyons are reported.



In the two figures above, a building array, realized for wind-tunnel experiments by investigators Robert Lawson, Michael Brown, David De Croix, and Robert Lee at the meteorological wind tunnel of US-EPA is shown.

One of the most difficult aspects to evaluate, in order to construct a database for full-scale simulations, is the turbulent effect created by the presence of obstacles (buildings) randomly distributed in the territory, as shown in figure below, where pollutants, driven by wind and passing through the canyons, draw very complex trajectories, often characterized by whirls of different size and shape.

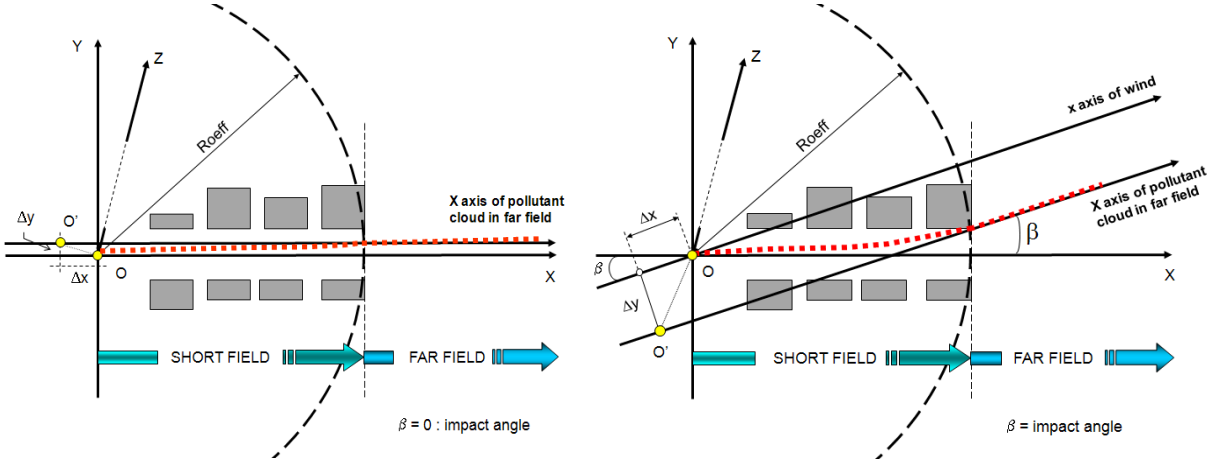




It is clear that all effects coming from the presence of whirls, obstacles, different layouts, different wind directions and velocities, different meteorological conditions, are absolutely impossible to be captured by a model, no matter if it has been created using Lagrangian, Eulerian or other approaches. The most significant way to proceed is to realize a database by processing experimental results, collecting the greater number of information for the main variables involved in that complex phenomenology, and then elaborate a series of algorithms and semi-empirical correlations for the simulation of real cases.

5.2 Impact angle

As previously anticipated, the impact angle β is the angle measured between buildings and wind directions, and in real applications it ranges from 0 to $\pi/3$.



The figure above shows two frequent situations in real calculations. The left scheme is the case in which $\beta = 0$, while the right one is more general and can be used as general reference for cases in which $0 < \beta \leq \pi/3$. Ro_{eff} is the effective homogenization radius.

Concerning β, a new parameter, called "*impact category*", ξ, is defined.

ξ determines two different classes, strongly linked to β as follows:

- $0 \leq \beta \leq \pi/6$ ➔ $\xi = 1$
- $\pi/6 < \beta \leq \pi/3$ ➔ $\xi = 2$

It is easy to understand that the first category is characterized by situations where pollutants run into canyons with smaller deviations and can go through them as far as wind speed is higher. In the second category we meet cases in which the impact with obstacles is stronger, therefore pollutants dispersion in short field is higher than in

previous one. It is clear that in these cases the building distribution, the occupancy index and the general short field situation represent predominant parameters to determine the situation in far field. In other words, it is absolutely important to locate, as best as possible, the end of short field.

6. ATMOSPHERIC STABILITY CLASS IN FAR FIELD

The calculation of homogenization radius leads to a clear-cut division of territory in short and far field but it is not sufficient to simulate pollutants behaviour. Also something more about atmospheric situation in the area in which accident happens must be known. The first step is to determine the atmospheric class according to meteorological variables, generally linked to solar radiation or nocturnal cloudiness, to vertical thermal gradient measured starting from ground level and to wind speed and direction.

The following six atmospheric stability classes should be put in relation with variables mentioned above:

- A: Extremely unstable
- B: Moderately unstable
- C: Slightly unstable
- D: Neutral
- E: Slightly stable
- F: Moderately stable

where class A is the most unstable or most turbulent, and class F the most stable or less turbulent. Alternatives to Pasquill-Gifford approach are the Monin-Obukhov length, the boundary layer height, and the wind speed to categorize the atmospheric turbulence. If the accident happens during the day, stability classes from A to D are the most propable. Stability classes from D to F are more probable for nocturnal events.

The calculation in the case of nocturnal events requires knowledge of cloudiness, not easily obtainable in the common monitoring stations. An alternative is to identify the class of atmospheric stability in function of the vertical thermal gradient.

PART 2: GUI AND WINDOWS TO INSERT DATA

FOR INPUT DECK PREPARATION

7. GUI AND CODE STRUCTURE

RADCAL-III mod. N code has been developed using MS Visual Basic Suite and C++.
This combination has resulted in the creation of a friendly dialog interface “user- code”, very attractive in terms of graphics and extremely clear in requests for input.

The aspect of the correction of trivial errors that the user may introduce under construction input is very well treated. If one of these errors is detected, the user is promptly notified and is also suggested how to proceed to correct them.

In every step of the phase of input data the user can go back and change the values previously entered. This is facilitated by the fact that, during the step of inserting data, some calculations are already performed and the data more congruent to proceed are indicated to the user. He can accept the suggestion (generally a range of data that prevents to bring the calculation to divergence is proposed) or continue with his own choices.

The output consists of a series of text files, easily transportable in Excel or equivalent application and graphically represented. RADCAL-III mod. N provides data of volume concentration of the airborne pollutants, in terms of C(x,y,z,t) and surface concentration of what is deposited at ground level, at terms C(x,y,t).

This allows to realize hundred of graphics with concentrations on the ground, at varying distances downwind of the source, graphics for a fixed time and with variable directions in x, y and z, concentrations at various heights from the ground and at various distances, downwind from the main x axis, or with reference to the main y axis and to its parallel axes located at increasingly large lateral distances from it.

Given all the possible combinations, it is difficult to describe in words the potential and the amount of information that can be derived from the graphical representation of the results.

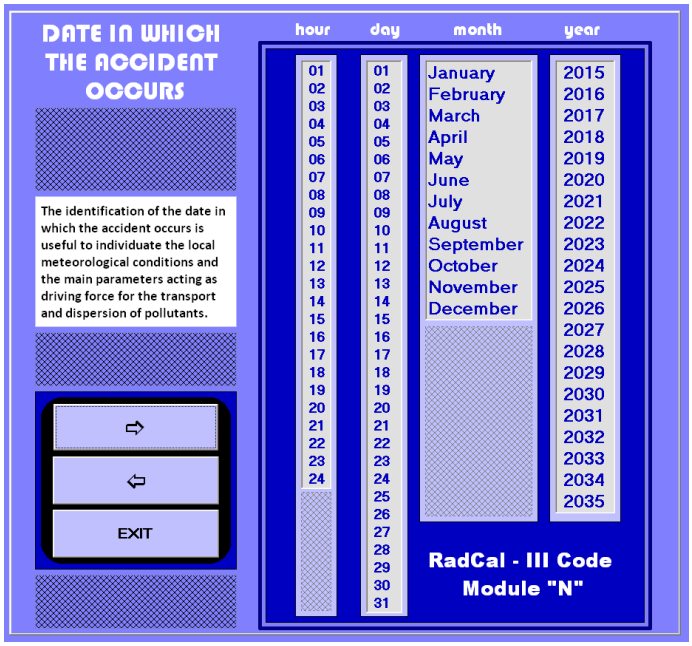
The best way to become expert users is to prepare a good input deck, perform calculations, and then proceed to post-processing, with the realization of all graphics necessary to better understand the aspects under investigation.

8. INPUT DECK STEPS

Here are reported only some of the many windows containing questions that the user must answer to prepare the input deck.

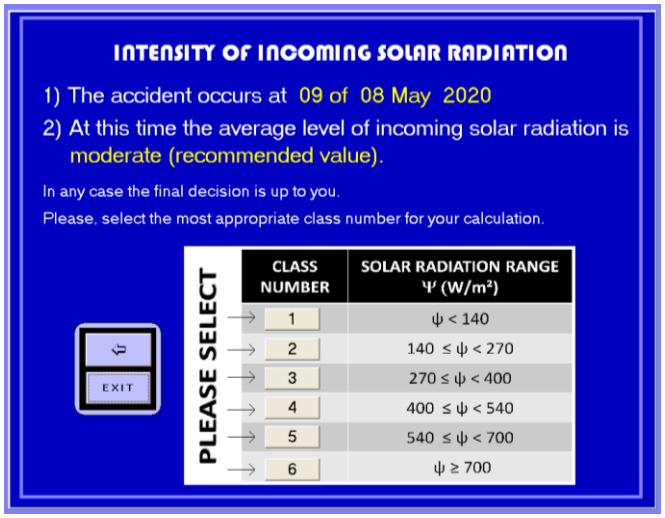
The first window is the welcome one, with general information about the code version and contacts in ENEA.

After some other windows, users must give information about the date in which accident occurs (hour, day, month and year).

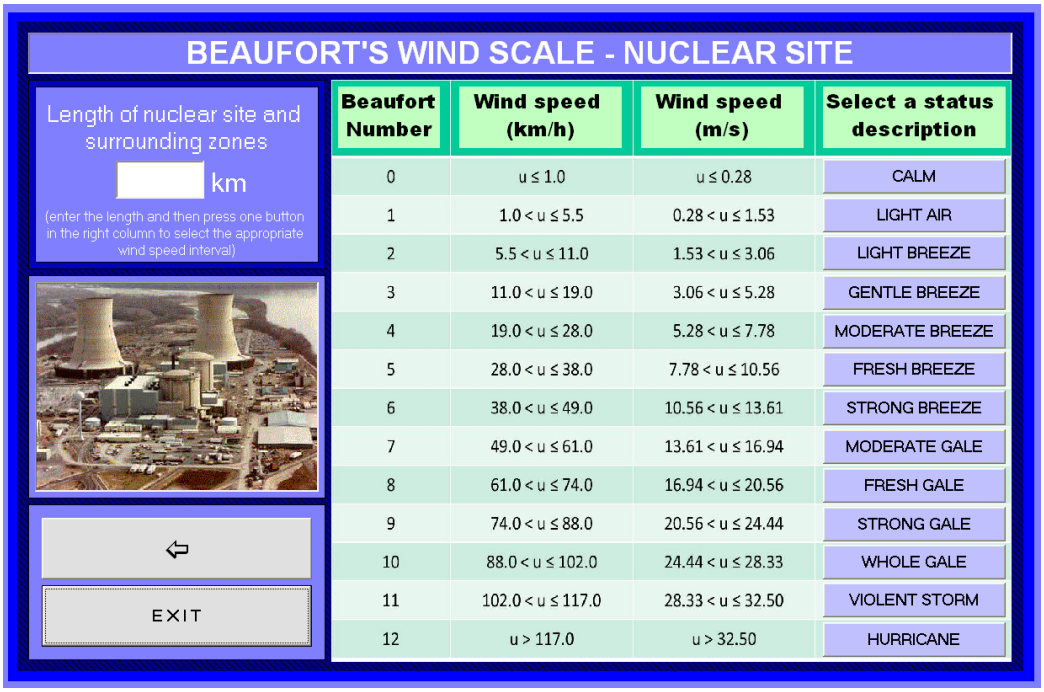


For example, we have assumed that the accident occurs at 9 am on 8 May 2020.

As it can be seen, in point 2 the code gives its information about the fact that the average level of incoming solar radiation at the indicated date (drawn from historical series in its internal meteorological database) is moderate.
Moderate means that users can select class number 3 or 4. This is the code suggestion, but in any case users are free to make their independent choice.

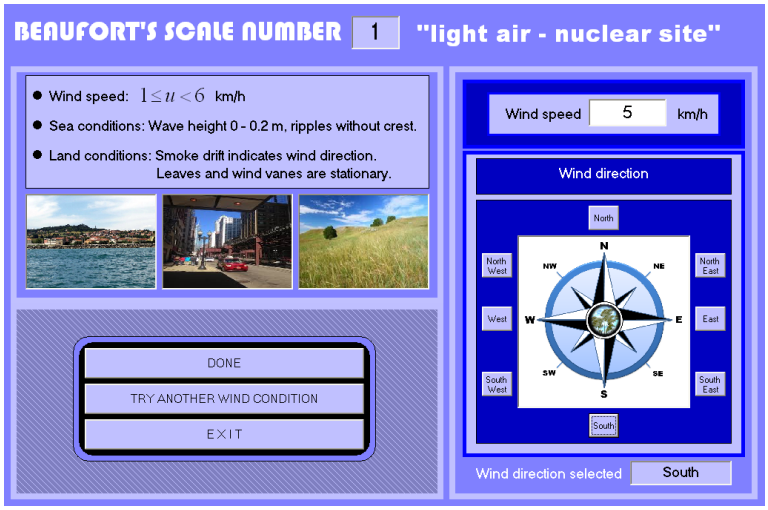


Another important windows is shown below. Here are requested information about the length in km of nuclear site and surrounding zones and a class of wind speed among those available making reference to Beaufort's wind scale.

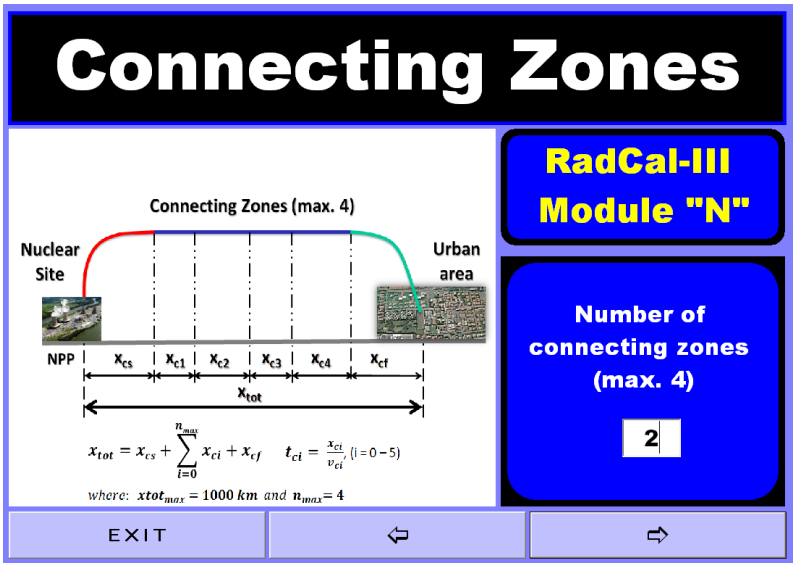


In this example, we have selected class number 1. It means that at the moment of accident the wind speed in the nuclear site was from 1 and 6 km/h. Our exact choice inside the selected interval is: 5 km/h, direction South.

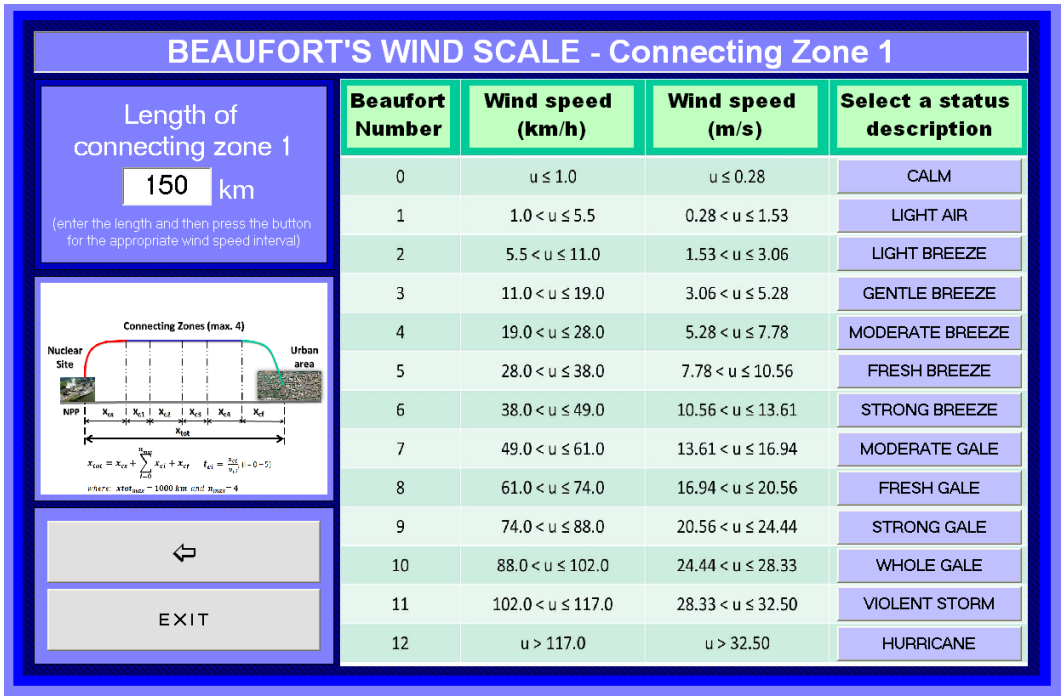
As we can see in the left part of window below, the code gives some information about sea and land conditions for this wind class. If users do not want to use this windows, they can press the button “Try another wind condition” and make corrections.

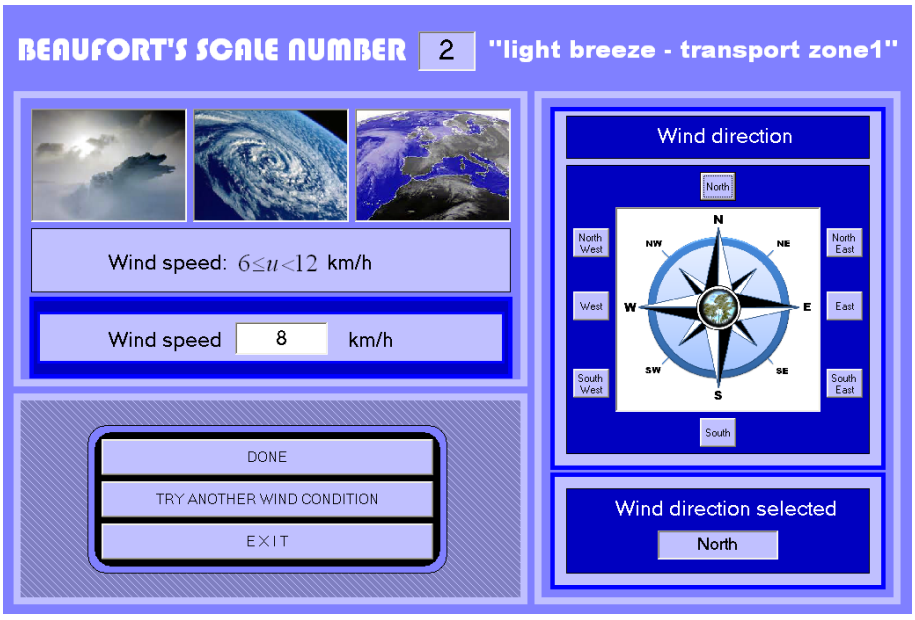


RADCAL-III mod. N is able to process four different connecting zones before arriving to the involved urban area. These zones are areas of transport, where the contaminants pass through, driven by local weather conditions, up to the urban area. Here we simulated two connecting zones.

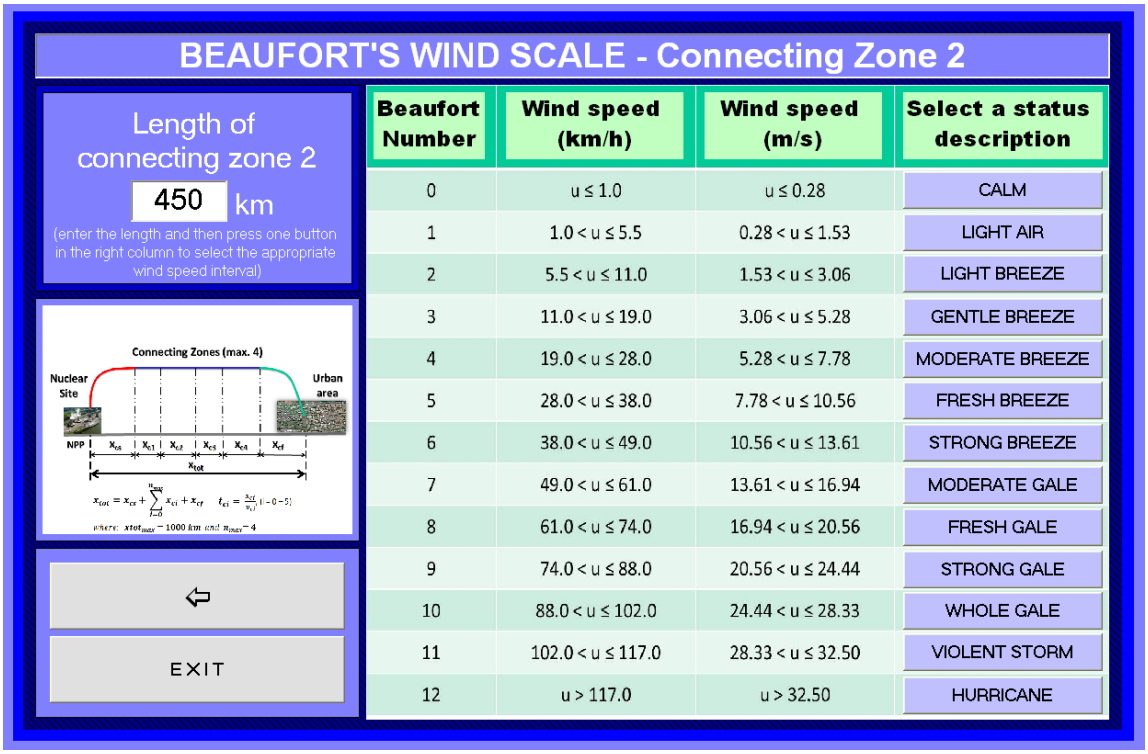


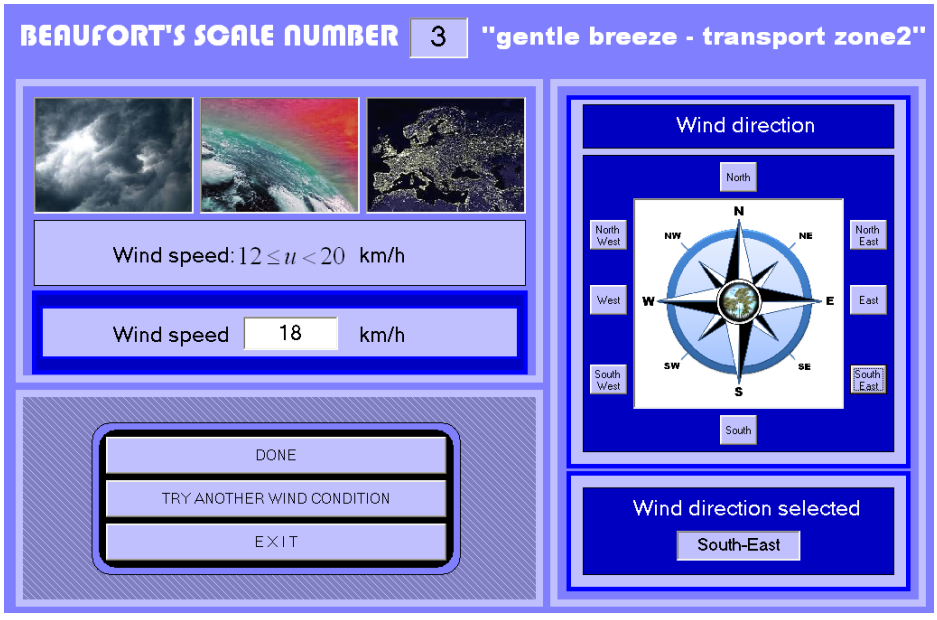
For each connecting zone it is necessary to give information about local weather conditions, as shown in next four windows.





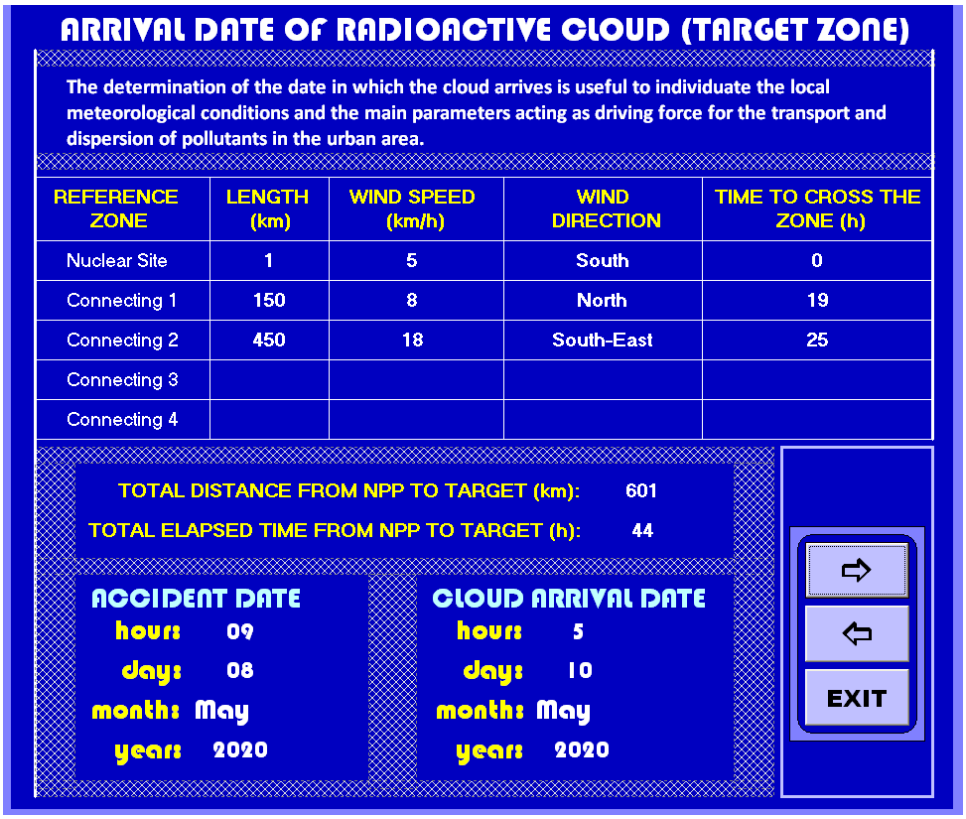
Here, for connecting zone 1, the length is 150 km, while the selected wind speed lies in Beaufort's scale n. 2 (our choice is 8 km/h, direction North).



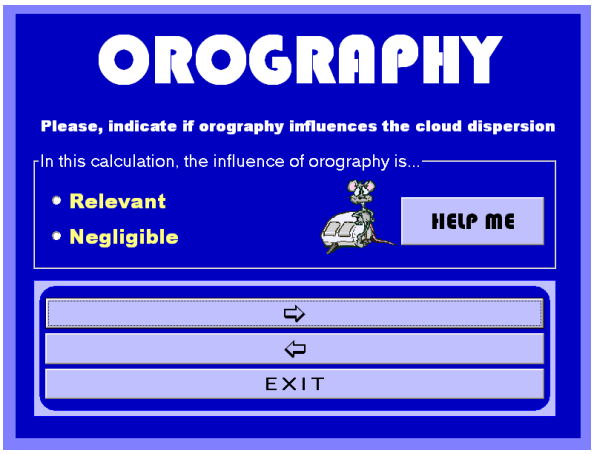


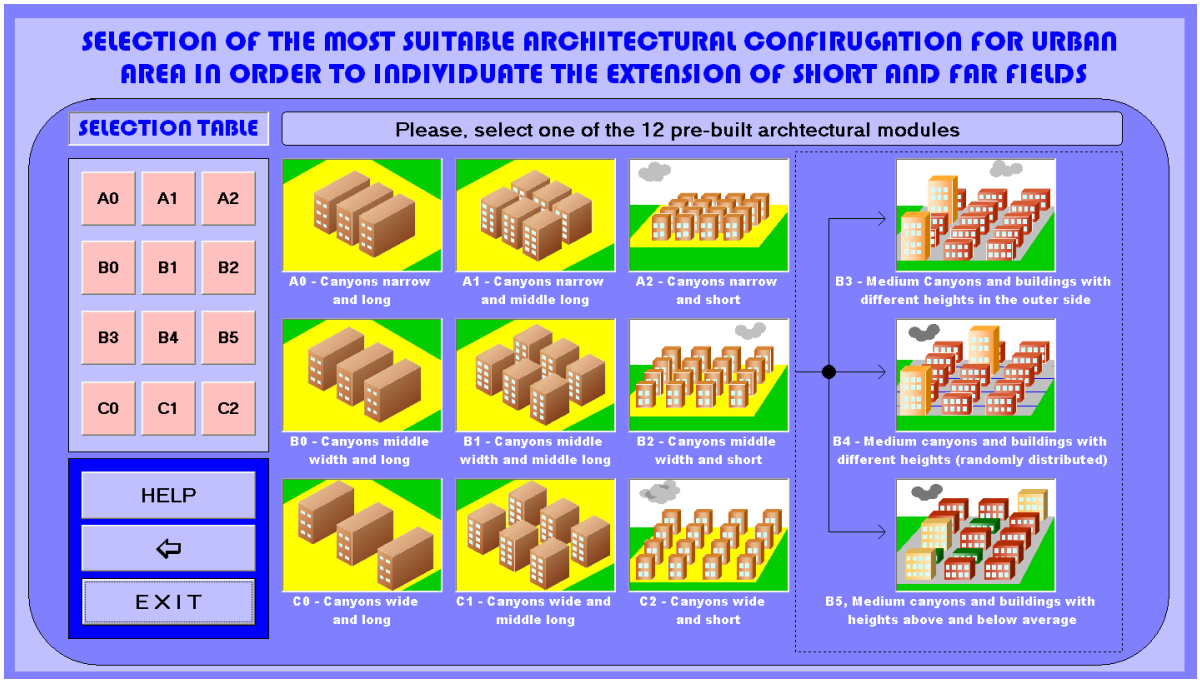
For connecting zone 2, the length is 450 km, and the selected wind speed lies in Beaufort's scal n. 3 (our choice is 18 km/h, direction South-East).

Using this information, the code is able to calculate the transit time in the connecting zones and therefore also the arrival date of the cloud in close proximity to the urban area involved.



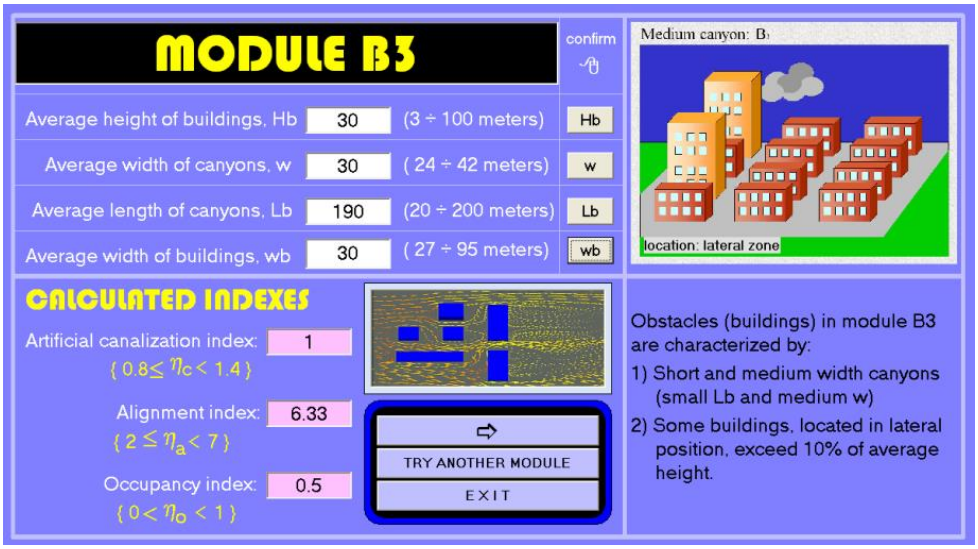
Some computer codes are not able to perform calculation considering the presence of obstacles and orography thus RADCAL-III mod. N provides to the user the opportunity to choose if he wants to proceed with calculations taking into account orography or considering it negligible. The second choice may be sometime useful to perform code-to-code comparisons.





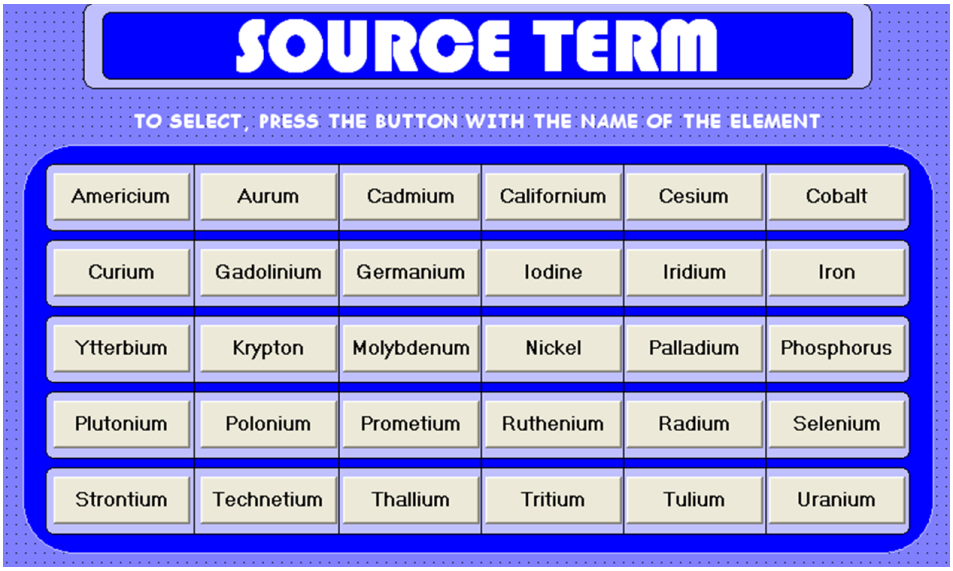
If the presence of obstacles in urban areas should be taken into account, then the window above is very useful. Users must provide information on the architectural structure of the urban area in order to take proper account of: a) the presence of canyons; b) the distribution of streets and buildings; c) meteorological and physical effects in short field.

In this section, the code provides a great help to the user, suggesting, step by step, what are the most appropriate ranges of building height, canyons width, and so on, in order to use one of the twelve pre-built architectural modules, able to represent in the best way the general layout of interest.



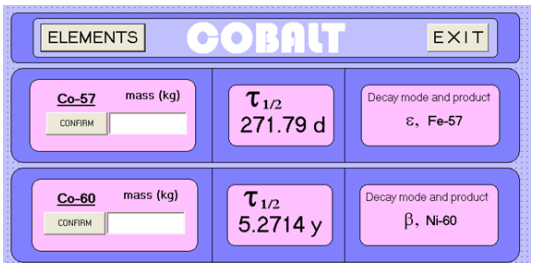
When all necessary data have been entered, RADCAL-III mod. N provides information on artificial canalization index, alignment index and occupancy index, as shown in the lower part of window above. If the architectural configuration does not meet expectations, users can go back and correct the input. In a similar way, as shown previously, users are requested to provide detailed information on the situation in the short and far field.

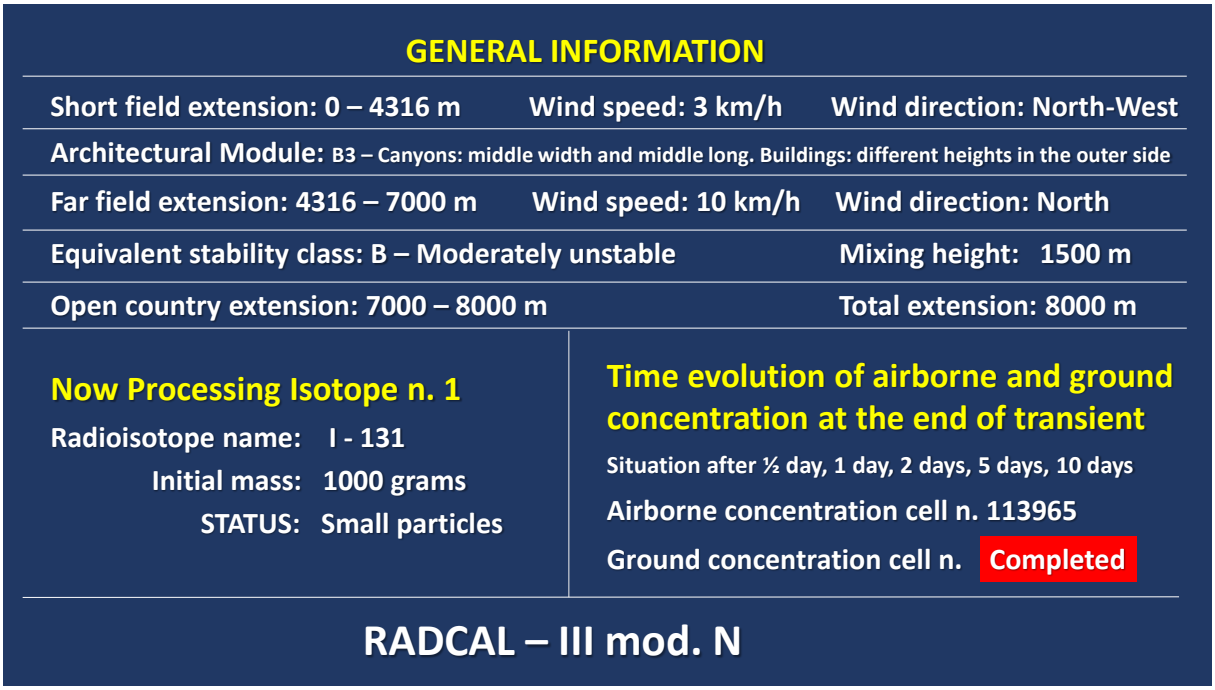
Many other windows will appear in sequence with the request for data and details in order to prepare the best possible input deck.



In addition, a certain number of information are requested to prepare the list of radioisotopes involved in the accident.

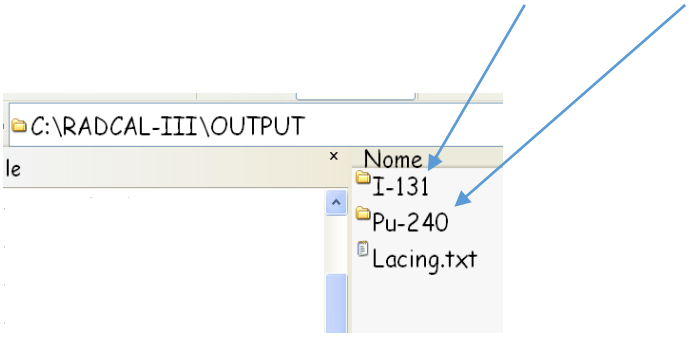
A great number of radioisotopes of several elements can be entered. The first step is to select the wanted element and to provide information, selecting the appropriate radioisotope.



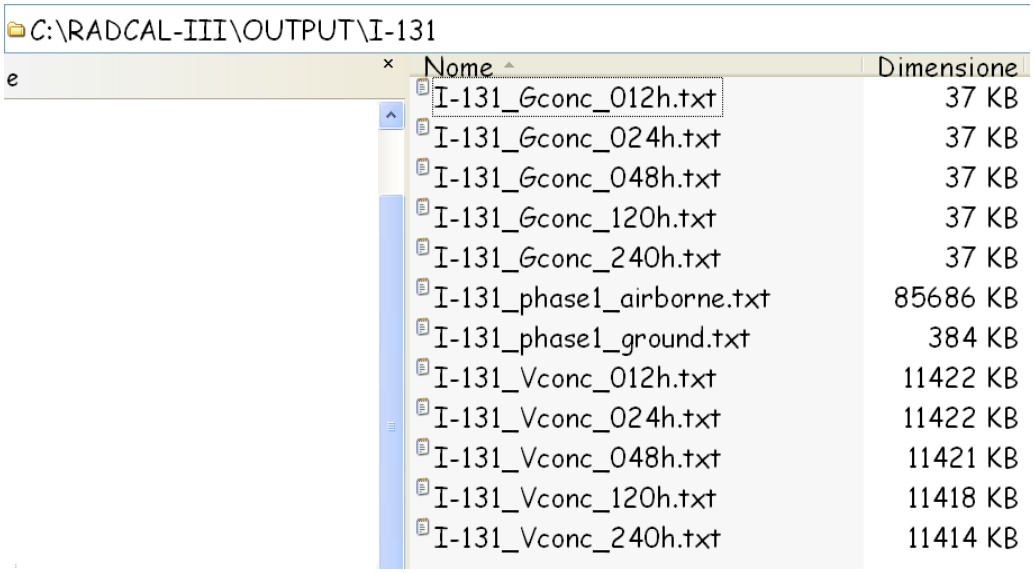


The window above is a snapshot made during a processing step of a calculation. It should be noted that during the calculation the set of information changes continuously. Many lines are updated also in graphic form and shown depending on what stage of processing is under evaluation: short field, far field or open country.

Finally, we report here an example of a list of files in the output folder at the end of the calculation. Here calculations for I-131 and Pu-240 have been simulated.



If, for example, one opens the directory in which the files relating to the I-131 are contained, this is one of the possible number of files prepared by RADCAL-III mod. N.



Filenames of the type: I-131_phase1_airborne.txt contain results of calculated volumetric concentrations (Bq/m^3) in air during the first phase, strongly characterized by transient conditions.

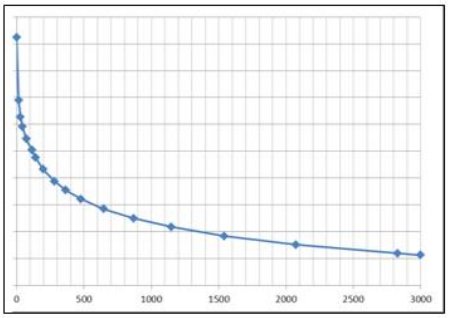
Filenames of the type: I-131_phase1_ground.txt contain results of calculated surface concentrations (Bq/m^2) at ground level during the first phase.

Filenames of the type: I-131_Vconc_012h.txt, 024h.txt, 048h.txt, 120h.txt and 240h.txt, contain results of calculated volumetric concentrations (Bq/m^3) in air after 12 hours, 1 day, 2 days, 5 days and 10 days.

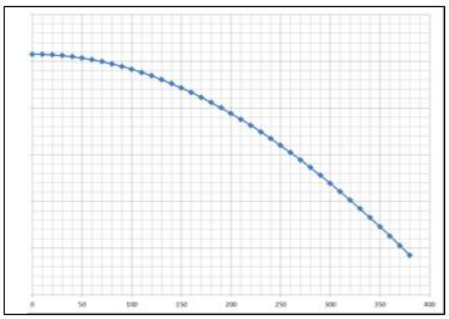
Filenames of the type: I-131_GVconc_012h.txt, 024h.txt, 048h.txt, 120h.txt and 240h.txt, contain results of calculated surface concentrations (Bq/m^2) at ground level after 12 hours, 1 day, 2 days, 5 days and 10 days.

If, for example, we refer to Cs-137, below are given three of the various possible hundreds of graphics (the quantity depends only on the will of the user) that can be prepared starting from the output files.

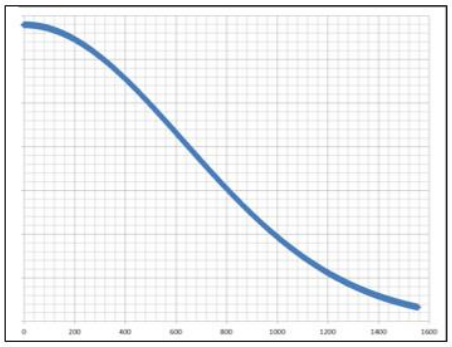
SOME RESULTS – Release of Cs-137



Concentration (Bq/m^3) in air (~ 1 m) at different distances x (downstream)



Concentration (Bq/m^3) in air at x=3000 m and for different distances (y) from main axis



Concentration (Bq/m^3) in air at x=3000 m and for different heights (z)

At the end of calculations, RADCAL-III gives the possibility to create a word file in which a short summary with all the most relevant input data entered are reported.

8. CONCLUSIONS

In this third year of PTR 2012-14, implementations of: a) IT systems; b) models with proper physical characteristics; c) several weather conditions; d) options; and e) strongly representative architectural pre-built modules, have been completed.

Phase-I is successfully concluded.

It is expected to initiate phase-II since the first year of PTR 2015-17, in order to start the validation process and conclude the work with the concrete availabilty of a very user-friendly and relatively fast calculation tool, and at the same time valid and reliable.